Volume 72B
Number 3
July–Sept. 1968

Mathematical Sciences

Formerly—
Mathematics and
Mathematical Physics

NOV 21 1968

UNIVERSITY LIBRARY

U.S. DEPARTMENT
OF COMMERCE

SECTION B

JOURNAL OF RESEARCH

NATIONAL BUREAU OF STANDARDS

Journal of Research

of the

National Bureau of Standards

B. Mathematical Sciences
(Formerly Mathematical and Mathematical Physics)

JULY–SEPT. • 1968

VOLUME • 72B

NUMBER • 3

Editor: Morris Newman

Associate Editors: John J. Sopka, F. W. Olver, and J. R. Edmonds

Publication dates: Mar. 10, June 10, Sept. 10, Dec. 10, 1968

JOURNAL OF RESEARCH

The National Bureau of Standards Journal of Research reports research and development in the fields of activity shown at right. Also included from time to time are survey articles on topics closely related to the Bureau's scientific and technical program.

The Journal is published in three separate sections as follows:

A. Physics and Chemistry

Contains papers of interest primarily to scientists working in these fields. Issued six times a year. Annual subscription: domestic, $6.00; foreign, $7.25. Single copy $1.00.

B. Mathematical Sciences

Presents studies and compilations designed mainly for the mathematician and the theoretical physicist. Issued quarterly. Annual subscription: domestic, $2.25; foreign, $2.75. Single copy 75c.

C. Engineering and Instrumentation

Reports research and development results of interest chiefly to the engineer and the applied scientist. Issued quarterly. Annual subscription: domestic, $2.75; foreign, $3.50. Single copy 75c.

NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards[1] was established by an act of Congress March 3, 1901. Today, in addition to serving as the Nation's central measurement laboratory, the Bureau is a principal focal point in the Federal Government for assuring maximum application of the physical and engineering sciences to the advancement of technology in industry and commerce. To this end the Bureau conducts research and provides central national services in three broad program areas and provides central national services in a fourth. These are: (1) basic measurements and standards, (2) materials measurements and standards, (3) technological measurements and standards, and (4) transfer of technology.

The Bureau comprises the Institute for Basic Standards, the Institute for Materials Research, the Institute for Applied Technology, and the Center for Radiation Research.

THE INSTITUTE FOR BASIC STANDARDS provides the central basis within the United States of a complete and consistent system of physical measurement, coordinates that system with the measurement systems of other nations, and furnishes essential services leading to accurate and uniform physical measurements throughout the Nation's scientific community, industry, and commerce. The Institute consists of an Office of Standard Reference Data and a group of divisions organized by the following areas of science and engineering:

Applied Mathematics—Electricity—Metrology—Mechanics—Heat—Atomic Physics—Cryogenics[2]—Radio Physics[2]—Radio Engineering[2]—Astrophysics[2]—Time and Frequency.[2]

THE INSTITUTE FOR MATERIALS RESEARCH conducts materials research leading to methods, standards of measurement, and data needed by industry, commerce, educational institutions, and government. The Institute also provides advisory and research services to other government agencies. The Institute consists of an Office of Standard Reference Materials and a group of divisions organized by the following areas of materials research:

Analytical Chemistry—Polymers—Metallurgy—Inorganic Materials—Physical Chemistry.

THE INSTITUTE FOR APPLIED TECHNOLOGY provides for the creation of appropriate opportunities for the use and application of technology within the Federal Government and within the civilian sector of American industry. The primary functions of the Institute may be broadly classified as programs relating to technological measurements and standards and techniques for the transfer of technology. The Institute consists of a Clearinghouse for Scientific and Technical Information,[3] a Center for Computer Sciences and Technology, and a group of technical divisions and offices organized by the following fields of technology:

Building Research—Electronic Instrumentation—Technical Analysis—Product Evaluation—Invention and Innovation—Weights and Measures—Engineering Standards—Vehicle Systems Research.

THE CENTER FOR RADIATION RESEARCH engages in research, measurement, and application of radiation to the solution of Bureau mission problems and the problems of other agencies and institutions. The Center for Radiation Research consists of the following divisions:

Reactor Radiation—Linac Radiation—Applied Radiation—Nuclear Radiation.

[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.
[2] Located at Boulder, Colorado 80302.
[3] Located at 5285 Port Royal Road, Springfield, Virginia 22151.

U.S. DEPARTMENT OF COMMERCE
C. R. Smith, Secretary
NATIONAL BUREAU OF STANDARDS
A. V. Astin, Director

Order all publications from the Superintendent of Documents
U.S. Government Printing Office, Washington, D.C. 20402.

Use of funds for printing this publication approved by the Director of the Bureau of the Budget (June 22, 1966).

JOURNAL OF RESEARCH of the National Bureau of Standards—Mathematical Sciences
Vol. 72B, No. 3, July–September 1968

Interaction in Multidimensional Contingency Tables: An Information Theoretic Approach[1,2]

H. H. Ku

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

and

S. Kullback

The George Washington University, Washington, D.C. 20006

(May 10, 1968)

The problem of interaction in multidimensional contingency tables is investigated from the viewpoint of information theory as developed by Kullback. The hypothesis of no rth-order interaction is defined in the sense of an hypothesis of "generalized" independence of classifications with fixed rth order marginal restraints. For a three-way table, with given cell probabilities π_{ijk}, the minimum discrimination information for a contingency table with marginals $p_{ij.}$, $p_{.jk}$, and $p_{i.k}$ is given by the set of cell probabilities $p^*_{ijk}=a_{ij}b_{jk}c_{ik}\pi_{ijk}$ where a_{ij}, b_{jk}, and c_{ik} are functions of the given marginal probabilities, that is, $\ln(p^*_{ijk}/\pi_{ijk})=\ln a_{ij}+\ln b_{jk}+\ln c_{ik}$, representing no second-order interaction. The minimum discrimination information statistic, asymptotically distributed as χ^2 with appropriate degrees of freedom is

$$2\Sigma_{ijk}x_{ijk}\ln x_{ijk}-2\Sigma_{ijk}x_{ijk}\ln x^*_{ijk}\geqq 0$$

where x_{ijk} are the observed cell frequencies and x^*_{ijk} are the "no interaction" cell frequencies uniquely determined by a simple convergent iteration process of the marginals on π_{ijk}. For lower order marginal restraints the usual independence hypotheses are generated when π_{ijk} are taken to be the cell probabilities under uniform distribution. It is shown that the set p^*_{ijk} satisfies definitions of no second order interaction in a $2\times2\times2$ table given by Bartlett and no interaction in a $r\times s\times t$ table by Roy and Kastenbaum, and is also related to that given by Good. Results of application to the analysis of some "classical" three-dimensional contingency tables are given, together with full details for two four-dimensional examples.

Key Words: Contingency tables; estimation of cell frequencies from marginals; generalized independence; hypothesis testing; information theory; interaction; second-order interaction.

Introduction

In the last decade, a series of related papers appeared in various publications on the analysis of multiway contingency tables. The topic of particular interest was that of the definition and treatment of higher-order interaction. Among these papers, we cite, for instance, Roy and Kastenbaum [1956],[3] Plackett [1962], Darroch [1962], Birch [1963], Good [1963], and Goodman [1964a,

[1] Presented by title to the Institute of Mathematical Statistics, Columbus, Ohio 23–25 March 1967 under the title Interaction in Multi-dimensional Contingency Tables; Abstract in Annals of Mathematical Statistics, Vol. 38, 297 (1967).

[2] Supported in part by the Air Force Office of Scientific Research, Office of Aerospace Research, United States Air Force, under Grant AF-AFOSR 932-65.

[3] Figures in brackets indicate the literature references at the end of this paper.

1964b]. Also related were The Estimation of Probabilities by Good [1965], two reports by Bhapkar and Koch [1965, 1966], and their recent publication in Technometrics [1968].

In these papers, various aspects of the problem were treated and solutions offered. Consequently, results given are usually concerned with individual parts of the problem, depending on the author's motivation and interest. We propose to show, that some of these results can be unified through the use of information theory. The formulation, comparisons, and proofs will be given in section 2, and applications to the analysis of multidimensional contingency tables in section 3, following a historical review in section 1. First, however, we shall give a brief description of the problem and the notations that will be used.

Consider a random sample of n independent observations, where each observation can be classified by m criteria of classifications, say: row (R), column (C), and depth (D), for instance. Suppose there are r categories in the row classification, c categories in the column classification, and d categories in the depth classification, then there are exactly $r \times c \times d$ cells in the three dimensional table. Each observation by definition must fall in one of the cells, say, the ijkth cell, with probability p_{ijk}, where $i = 1, 2, \ldots, r, j = 1, 2, \ldots, c, k = 1, 2, \ldots, d$, are the subscripts relating the cell to the categories in the row, column, and depth classifications respectively.

Let x_{ijk} represent the observed frequency of the ijkth cell in the sample, so that $\Sigma_{ijk} x_{ijk} = n$. Then we have summarized the data in the form of a three-way contingency table with cell probabilities p_{ijk}, $\Sigma_{ijk} p_{ijk} = 1$.

Summing over categories over one classification or two classifications, we obtain two-way and one-way marginal tables respectively, or in symbols:

$$x_{ij.} = \Sigma_k x_{ijk}, \qquad x_{i..} = \Sigma_j x_{ij.} = \Sigma_{jk} x_{ijk},$$

and the like. Corresponding to these marginals frequency tables, we have similar marginal tables for the probabilities.

In the analysis of contingency table we are usually interested in the relationship between one classification and one or more of the other classifications. Suppose the row classification represents the response of an experiment on animals, the column classification types of treatment, and the depth classification a distinguishable characteristic of the sampled individuals, sex, for instance. Then in many respects the hypotheses of interest are analogous to those of independence and correlation in normal multivariate analysis, e.g.,

1. Response is independent of treatment, or

$$H_0 : p_{ij.} = p_{i..} p_{.j.}.$$

This case corresponds to simple correlation. That is, H_0 corresponds to the hypothesis that response and treatment are uncorrelated.

2. Response is independent of treatment and sex, or

$$H_0 : p_{ijk} = p_{i..} p_{.jk}.$$

This case corresponds to multiple correlation.

3. Response is independent of treatment, given the sex, or

$$H_0 : p_{ijk} = \frac{p_{i.k} p_{.jk}}{p_{..k}}.$$

This case corresponds to partial correlation.

Of course not all contingency tables can be interpreted in such a straightforward manner. In some cases all three classifications can be considered as responses; then we may be interested in the independence or associations among these responses. In other cases a classification may

be viewed either as a factor or a response. For convenience, we may group all the concepts of association, dependence, etc., under the general term of interaction. No interaction between treatment and sex appears to be a more acceptable phrase than independence between treatment and sex since independence is usually reserved to express the relationship between two random variables. We may also say that the interaction between response and treatment does not interact with sex, meaning the degree of association between response and treatment is the same for both sexes.

Here we come to grips with a concept which gives rise to the idea of second-order interaction (sometimes called a three-factor interaction when applied to a three-way table). The definition, method of analysis, and the interpretation of the second-order and higher-order interactions have been the source of controversy for a number of years. It is probably worthwhile to review the historical development of the problem and to summarize the various schools of thought on the subject to gain a proper perspective for the present treatment. A brief account will be given in the next section.

1. Historical Background

1.1. Formulation of the No-Interaction Hypothesis

The first use of the "no second-order interaction" hypothesis as relating to a $2\times2\times2$ contingency table was due to Bartlett [1935]. The concept remained dormant for a number of years. Lewis [1962], in his excellent review on the subject, lamented that ". . . there is still no coordinated information available, and the treatment of these tables is still widely neglected in standard text books."

Bartlett's definition was mainly intuitive. Since then, there have been several attempts to arrive at a logical, consistent, and intuitively acceptable definition that could be derived from within a wider framework of hypothesis formulation. The main lines of thought can be grouped into the following classifications:

1. Bartlett's original definition and its extensions.
2. Simpson, Plackett, and Darroch's formulations based on symmetrical functions of the cell probabilities.
3. Good's definition based on maximum entropy and Goodman's modification.

1.2. Bartlett's Definition and Its Extension by Roy and Kastenbaum

Bartlett defined his term, formulated the hypothesis, proposed the statistic and suggested a method for the solution in less than 25 lines! To use the author's words, "The testing of independence in a 2×2 table with fixed marginal totals, may be regarded as testing the significance of the interaction between the two classifications . . .. Corresponding to the hypothesis to be tested in an ordinary fourfold table (i.e., a 2×2 table) of observed numbers n_1, n_2, n_3, n_4 that $p_1p_4=p_2p_3$, we require to test the hypothesis (of no second-order interaction) that

$$p_1p_4p_6p_7=p_2p_3p_5p_8." \tag{1.1}$$

$$\text{(i.e., } p_{111}p_{122}p_{212}p_{221}=p_{112}p_{121}p_{211}p_{222}.)$$

Thus for a 2×2 table with fixed marginal totals, Bartlett's definition of no first-order interaction implies and is implied by independence of the two classifications. Furthermore, he assumed that the cross-product ratio type of hypothesis can be extended to define second-order interaction for $2\times2\times2$ tables. It is remarkable that his definition remains the preferred one to this date and the same hypothesis has been arrived at by others through different approaches.

Bartlett's definition, however, becomes complicated when the categories within a classification are more than two—a difficulty acknowledged by him in the latter part of his paper. Proper inter-

pretation of results of the test also becomes difficult. Moreover, the solution requires lengthy iterative computation for the solution of $(r-1)(c-1)(d-1)$ simultaneous third degree equations, where r, c, and d are respectively, the number of categories in the row (R), column (C), and depth (D) classifications.

Norton [1945] extended Bartlett's definition to $2\times2\times d$ tables, and devised an iterative procedure for solving these systems of equations. Roy and Kastenbaum [1956], commenting that "Bartlett's and Norton's papers do not give any indication of the mechanism behind the formula for the hypothesis of no interaction . . .", derived a set of "no interaction constraints" in an $r\times c\times d$ table in the form of

$$\frac{p_{rcd}p_{ijd}}{p_{icd}p_{rjd}}=\frac{p_{rck}p_{ijk}}{p_{ick}p_{rjk}} \quad \text{for } \begin{matrix} i=1,2,\ \ldots,(r-1) \\ j=1,2,\ \ldots,(c-1) \\ k=1,2,\ \ldots,(d-1). \end{matrix} \tag{1.2}$$

The set of constraints reduces to (1.1) for a $2\times2\times2$ table.

The "mechanism" used by Roy and Kastenbaum is based on the fact that the two hypotheses

$$H_1: p_{i\cdot k}=p_{i\cdot\cdot}p_{\cdot\cdot k}$$

$$H_2: p_{ij\cdot}=p_{i\cdot\cdot}p_{\cdot j\cdot}$$

will not usually imply

$$H: p_{ijk}=p_{i\cdot\cdot}p_{\cdot jk}$$

in a three-way contingency table. The "no interaction" hypothesis is required to generate the set of constraints such that these constraints, when superimposed on $H_1\cap H_2$ should imply H. The result is the set of constraints in (1.2). In contrast to Bartlett, Roy and Kastenbaum called (1.2) the hypothesis of "no interaction" or "no first-order interaction." The extension of this concept to the hypothesis of "no second-order interaction" in a four-way table was only indicated in their paper.

1.3. Simpson, Plackett, and Darroch's Formulation

Simpson [1951] required the definition of "no second-order interaction" to be symmetrical with respect to the three attributes of a $2\times2\times2$ table. If some function $\psi(p_{111}, p_{121}, p_{211}, p_{221})$ is chosen to measure the association of classifications R and C in D, then the function must be such that the equation

$$\psi(p_{111}, p_{121}, p_{211}, p_{221})=\psi(p_{112}, p_{122}, p_{212}, p_{222})$$

implies and is implied by the equations

$$\psi(p_{111}, p_{211}, p_{112}, p_{212})=\psi(p_{121}, p_{221}, p_{122}, p_{222})$$

and

$$\psi(p_{111}, p_{121}, p_{112}, p_{122})=\psi(p_{211}, p_{221}, p_{212}, p_{222}).$$

He showed that the function $\psi=\frac{p_{121}p_{211}}{p_{111}p_{221}}$ or the cross-product ratio used by Bartlett, satisfies this requirement. Hence, Bartlett's definition for a $2\times2\times2$ table was accepted. The uniqueness of this function was not discussed.

In a footnote to Simpson's paper, the editor suggested that "This paper should be read in conjunction with the following paper by H. O. Lancaster." Lancaster [1951] defined the second-

order interaction by the partition of the chi-square statistic X^2; i.e., it is defined as the difference between the total X^2 for testing complete independence of the three classifications, and the sum of the three components corresponding to tests for independence in each of the three marginal tables.

Plackett [1962] compared Simpson's definition with Lancaster's definition [1951] and showed that the latter does not always satisfy the condition of symmetry. He accepted Roy and Kastenbaum's definition given in (1.2) for an $r \times c \times d$ table, and extended the analysis of log-frequencies [Woolf 1955] to such tables as an alternative method of analysis which is computationally easier than the solution of $(r-1)(c-1)(d-1)$ simultaneous equations of the third degree.

Darroch [1962] made an explicit comparison of the definitions of interaction in multiway contingency tables and in the analysis of variance. He found that there are resemblances between the two definitions but "that interactions in contingency tables enjoyed only a few of the fortuitously simple properties of interactions in the analysis of variance." The main point he made (also made by Roy and Kastenbaum) was that a natural symmetrical definition of "no second-order interaction"

$$p_{ijk} = \frac{p_{\cdot jk} p_{i\cdot k} p_{ij\cdot}}{p_{i\cdot\cdot} p_{\cdot j\cdot} p_{\cdot\cdot k}} \tag{1.3}$$

necessarily imposes constraints on the marginal probabilities $p_{ij\cdot}$, $p_{\cdot jk}$, $p_{i\cdot k}$, i.e.,

$$\Sigma_k p_{ijk} = p_{ij\cdot} = \frac{p_{ij\cdot}}{p_{i\cdot\cdot} p_{\cdot j\cdot}} \Sigma_k \frac{p_{i\cdot k} p_{\cdot jk}}{p_{\cdot\cdot k}},$$

or

$$\Sigma_k \frac{p_{i\cdot k} p_{\cdot jk}}{p_{\cdot\cdot k}} = p_{i\cdot\cdot} p_{\cdot j\cdot}$$

for all i, j, and the like. This is of course undesirable since the condition for "no second-order interaction" should relate p_{ijk} to any given set of marginal probabilities and should not place restrictions on the latter [cf. p. 172 Kullback 1959].

Consequently Darroch defined a "perfect three-way table" as one for which condition (1.3), and the resulting restraints on the marginal probabilities, are satisfied exactly. He concluded further that "in imperfect tables it is not possible to express p_{ijk} in terms of simple functions of $p_{ij\cdot}$, $p_{i\cdot k}$, and $p_{\cdot jk}$ when there is no second-order interaction." The existence and uniqueness of the set p_{ijk} as the solution of (1.2) for any given set of mutually consistent marginal probabilities was conjectured for $r \times c \times d$ tables and proved for the $2 \times 2 \times 2$ case. The search for a simple formulation in terms of parameters which are implicitly defined by the marginal probabilities led Darroch to define

$$p_{ijk} = \mu \alpha_{jk} \beta_{ki} \gamma_{ij}$$

where

$$\Sigma_k \alpha_{jk} = \Sigma_i \beta_{ki} = \Sigma_j \gamma_{ij} = 1,$$

and

$$\mu \Sigma_{ijk} \alpha_{jk} \beta_{ki} \gamma_{ij} = 1;$$

and showed that

$$\mu \doteq 1,\ \alpha_{jk} \doteq \frac{p_{\cdot jk}}{p_{\cdot j\cdot}},\ \beta_{ki} \doteq \frac{p_{i\cdot k}}{p_{\cdot\cdot k}},\ \text{and}\ \gamma_{ij} \doteq \frac{p_{ij\cdot}}{p_{i\cdot\cdot}}.$$

Since there is no solution in closed form to the maximum likelihood equations for the parameters under hypothesis of no second-order interaction, unless the observed table happens to be perfect, Darroch suggested an iterative solution and gave a numerical illustration using the example given by Kastenbaum and Lamphiear [1959].

It is of interest to note that Darroch suggested the likelihood ratio test based on

$$Z_{RCD}=2\Sigma_{ijk}n_{ijk}\ln\left(\frac{n_{ijk}}{n\hat{\mu}\hat{\alpha}_{jk}\hat{\beta}_{ki}\hat{\gamma}_{ij}}\right)$$

which is asymptotically distributed as χ^2 with $(r-1)\times(c-1)\times(d-1)$ degrees of freedom.

Birch [1963] accepted (1.2) as the definition of no second-order interaction in a 3-way table and discussed maximum likelihood estimation of expected frequencies for many-way tables under different hypotheses. He also proved the conjecture by Darroch that the expected frequencies in a three-way table are uniquely given by the marginal totals if the expected frequencies are known to be positive and to satisfy the hypothesis of no second-order interaction. Thus, given any set of positive integers n_{ijk} he showed that there is one and only one set of positive numbers n^*_{ijk} that satisfies the equations

$$n^*_{ij.}=n_{ij.},\ n^*_{i.k}=n_{i.k},\text{ and }n^*_{.jk}=n_{.jk},$$

and also the conditions given by the no second-order interaction hypothesis expressed by (1.2).

1.4. Good's Formulation

The formulations of the hypothesis of no second-order interaction summarized up to now are basically extensions of Bartlett's. Justifications for such formulations are given in a number of ways: (1) residually as the difference between the independence of one classification (R) with the other two classifications (CD) and the two independence hypotheses ($R\times C$) and ($R\times D$); (2) by symmetry requirements; (3) by analogy with analysis of variance. Lancaster [1951] also proposed a formulation based strictly on the analogy of the partition of χ^2 to the analysis of variance. The shortcomings of his method were discussed by Lewis [1962] and Plackett [1961] and will not be repeated here.

Good [1963] proposed to use the principle of maximum entropy as a heuristic principle for the generation of null hypotheses, with main application to m-dimensional contingency tables. Three versions of this principle are given in his paper. We quote here his Principle of Minimal Discriminability: "Let X be a random variable whose distribution is subject to some set of restraints. Suppose that, before the restraints were known, there was some distribution that seemed reasonable to entertain as a null hypothesis, called an initially ausgezeichnet hypothesis. This hypothesis is perhaps refuted by the constraints. Then, in view of the restraints, entertain the null hypothesis that, if true, can be discriminated from the ausgezeichnet hypothesis at the minimum rate, i.e., for which the expected weight of evidence per observation is least."

Numerous examples and theorems are given in Good's paper. By using his principle, it is shown that for an m-dimensional $2\times2\times\ \ldots\times2$ contingency table $(p_i)=(p_{i_1i_2\ \ldots\ i_m})$, $i_1, i_2, \ldots, i_m=0$, 1, and with all the marginal probabilities down to $(m-1)$-way assigned, the null hypothesis to be tested is

$$\prod_{i}^{|i|\text{ even}}p_i=\prod_{i}^{|i|\text{ odd}}p_i$$

where $|i|=i_1+i_2+\ \ldots+i_m$. The expression reduces to (1.1) when $m=3$.

Good also generalized the definition to that of no rth-order and all higher-order interactions in an m-dimensional contingency table with a complete set of rth-order restraints by means of discrete Fourier transforms of the logarithms of probabilities. However, the interactions so defined are usually complex valued unless the categories within each classification are equal to two. Goodman

[1964] followed the definition by Good but proposed a test that yields real valued interactions. Goodman's proposed test is based on Wald's criterion [1943] and unrestricted maximum likelihood estimates, and is essentially an extension of the tests proposed by Plackett [1962] and Woolf [1955].

While Good's and Goodman's formulations and tests of no-interaction hypotheses are entirely general, physical interpretations of their meanings became extremely difficult, if not impossible, for interactions higher than the second, in which case these interactions reduce to the ones discussed before. Bhapkar and Koch [1965, 1966, 1968] outlined the models, tests, and interpretations of the hypothesis of no interaction in three-dimensional and four-dimensional contingency tables in great detail, and compared results of using different statistics, all based on Wald's criterion, for several numerical examples.

1.5. Conditions Essential to a Definition of Hypothesis of No Interaction in Multidimensional Contingency Tables

Based on the above review of treatments of higher-order interactions, it appears that several basic and related concepts are important in the formulation of its definition:

a. The Fixed Marginal Totals

In fact, to talk about the rth-order interaction in an m-way table, the r-way marginals must be considered fixed; for otherwise we would be considering a less restricted hypothesis which includes the no-interaction hypothesis as a subhypothesis. This concept was implied in Bartlett's and Roy's definition, and explicitly stated in Good's definition. Darroch and Birch also assumed fixed marginals. Goodman and Bhapkar, on the other hand, did not make such a demand on their definitions, and hence their formulations are less desirable in the sense that their interaction *does not measure the interaction as* given by the data, but that possibly for another set of data with somewhat different marginal totals.

b. The Requirements of Symmetry

This requirement is a "logically attractive" condition as stated by Simpson, and demands that the statistic be invariant upon relabeling of the classifications. This requirement is again satisfied by all investigations with the exception of Goodman, and Bhapkar and Koch, who maintained that the symmetry requirement is not necessarily desirable for certain physical interpretations.

c. Unique Set of Cell Probabilities ($p_i > 0$)

The no-interaction hypothesis, which is presumably the last hypothesis to be tested in a hierarchy of hypotheses, should determine the cell probabilities uniquely. This condition was conjectured by Darroch for his formulation of the no second-order interaction hypothesis and shown to be true by Birch and Good. A measure of deviations of the data from this set of cell probabilities would therefore be a measure of interaction.

d. Additivity of the Statistics

The "mechanism" used by Roy and Kastenbaum in their definition of no interaction demands that H_1 (R is independent of C)$\cap H_2$ (R is independent of D)$\cap H_I$ (no interaction) implies H (R is independent of CD). The same requirement was also discussed by Birch [1963]. In general, if a more restrictive hypothesis can be considered as the intersection of several less restrictive hypotheses, it would be logical and desirable to require the test statistics for the component hypotheses to sum up to that of the more restrictive hypothesis. This requirement is not fulfilled by the usual X^2 statistic except in an asymptotic sense. The additive analysis of component variation, similar to that of analysis of variance, is a desirable feature of information analysis as noted by Lewis [1962].

2. Interaction from the Viewpoint of Information Theory

2.1. The Minimum Discrimination Information Statistic (m.d.i.s.)

In the analysis of contingency table data, two major types of hypotheses are usually postulated and tested. One is a test of the cell frequencies of an observed sample table against known or given probabilities of a table of the same size, the other is a test of the structural relationships that seem reasonable among the classifications, e.g., association or independence among responses, homogeneity of response over several categories of a factor, etc.

In Kullback [1959], and two papers by Kullback, Kupperman, and Ku [1962a, 1962b], a number of useful tests for contingency tables based on the notion of information theory are given for hypotheses which can be expressed explicitly as functions of specified marginal probabilities. The minimum discrimination information statistic, m.d.i.s., was suggested as the test statistic which, in its simplest form for a two-way contingency table, can be expressed as

$$2n\hat{I}(p:\pi)=2\Sigma_{ij}x_{ij}\ln\frac{x_{ij}}{n\pi_{ij}}, \tag{2.1}$$

where π_{ij} is the probability of an observation from the ith row and jth column of the table under the null hypothesis, $\Sigma_{ij}\pi_{ij}=1$, x_{ij} is the observed frequency of occurrence in the corresponding cell, $\Sigma_{ij}x_{ij}=n$, and ln is the natural logarithm. 0 ln 0 is defined as zero.

Similarly, the m.d.i.s. for the test of independence between the row and column classifications, i.e., $\pi_{ij}=\pi_{i.}\pi_{.j}$, is shown to be

$$2n\hat{I}(p:\pi)=2\Sigma_{ij}x_{ij}\ln\frac{x_{ij}}{\dfrac{x_{i.}x_{.j}}{n}}, \tag{2.2}$$

where $x_{i.}=\Sigma_j x_{ij}$, $x_{.j}=\Sigma_i x_{ij}$, are the row and column marginal frequencies of the two-way table.

We may consider either of the two tests given by (2.1) and (2.2) to be a comparison of the observed frequencies against a set of frequencies in a constructed table represented by $x^*_{ij}=np^*_{ij}$, where $\{p^*_{ij}\}$ is the set of cell probabilities that "most" resembles $\{\pi_{ij}\}$ subject to certain marginal probability restrictions. In fact, the set of $\{p^*_{ij}\}$ can be obtained by minimizing the discrimination information

$$2I(p:\pi)=2\Sigma_{ij}p_{ij}\ln\frac{p_{ij}}{\pi_{ij}} \tag{2.3}$$

subject to these restrictions. For the case considered under (2.1), the minimum value is zero for $p^*_{ij}=\pi_{ij}$, the restriction $\Sigma_{ij}np^*_{ij}=n$ is always fulfilled. For the case (2.2), the minimum value of (2.3) is attained for $p^*_{ij}=p_{i.}p_{.j}$, with the restriction $np_{i.}=x_{i.}$, and $np_{.j}=x_{.j}$, as shown in Kullback et al. [1962b].

It would clearly be desirable if this concept could be extended to the formulation of second-order and higher-order interactions. Here, however, we encounter essentially the same difficulties as discussed by Darroch, i.e., these interaction hypotheses cannot be formulated in terms of explicit functions of the marginal probabilities such that these functions also satisfy all the fixed marginal total restraints. To resolve these difficulties, we need to give a number of new results with information theoretical background due to Ireland and Kullback [1968] in conjunction with their study of an estimation problem first considered by Deming and Stephan [1940]. We shall summarize these results in the next section and show how they may be applied to give a unified approach to the analysis of interactions in multidimensional contingency tables.

2.2. Summary of Current Results

In the following we shall present a number of current results in the form of three theorems. Proofs for theorems 2.1 and 2.2 using properties of the minimum discrimination information are given in Ireland and Kullback [1968], and will not be repeated here. The use and interpretations of these theorems in our case for the purpose of hypothesis testing, however, are quite different from that of their paper which essentially treats a problem in estimation. These differences will be discussed and appropriate modifications to the statement of these theorems incorporated.

THEOREM 2.1. *Given a contingency table* $\{\pi_{ij}\}$, $i=1, 2, \ldots, r$, $j=1, \ldots, c$, $\pi_{ij}>0$, $\Sigma_{ij}\pi_{ij}=1$. *Consider all contingency tables* $\{p_{ij}\}$ *of the same dimension such that the marginal probabilities* $p_{i\cdot}=\Sigma_j p_{ij}$ *and* $p_{\cdot j}=\Sigma_i p_{ij}$ *are given and fixed. Then the minimum value of the discrimination information*

$$I(p:\pi)=\Sigma_{ij}p_{ij}\,ln\,\frac{p_{ij}}{\pi_{ij}} \tag{2.4}$$

is attained for $p_{ij}=p^*_{ij}=a_i b_j \pi_{ij}$ *where the* a_i*'s and* b_j*'s are determined subject to the marginal probability restrictions.*

Deming and Stephan [1940] considered the problem of estimation of cell probabilities from a sample of observations in an $r\times c$ table for which the population marginal probabilities $p_{i\cdot}$ and $p_{\cdot j}$ are known and fixed. Hence if we use the maximum likelihood estimates of the cell probabilities, $\pi_{ij}=n_{ij}/n$, which do not necessarily satisfy these marginal restraints, then the question can be posed "What is the p_{ij} distribution satisfying these restraints and also 'closest' to the observed sample in some sense?" Deming and Stephan [1940] suggested using estimates that minimized

$$(X')^2=\Sigma_{ij}(n_{ij}-np_{ij})^2/n_{ij}. \tag{2.5}$$

Ireland and Kullback [1968] suggested minimizing the discrimination information (2.4) which generates RBAN estimators, as does Deming and Stephan's procedure.

We note that π_{ij} is not specified in the theorem. If, instead of letting $\pi_{ij}=n_{ij}/n$, we use π_{ij} to represent the cell probabilities of some reasonable hypothesis which we are interested in, or the ausgezeichnet hypothesis in the sense of Good, then the p^*_{ij} distribution will represent the distribution that is "closest" to this hypothesized distribution subject to the marginal restraints in the sense of minimum discrimination information or "minimal discriminability". For instance, if $\pi_{ij}=\pi_{i\cdot}\pi_{\cdot j}$, or the hypothesis of independence of row and column classifications, then by theorem 2.1,

$$\begin{aligned} p^*_{ij}&=a_i b_j \pi_{ij},\\ p_{i\cdot}&=\Sigma_j p^*_{ij}=a_i\Sigma_j b_j\pi_{ij},\\ p_{\cdot j}&=\Sigma_i p^*_{ij}=b_j\Sigma_i a_i\pi_{ij}, \end{aligned}$$

and

$$p^*_{ij}=\frac{p_{i\cdot}}{\pi_{i\cdot}\Sigma_j b_j\pi_{\cdot j}}\cdot\frac{p_{\cdot j}}{\pi_{\cdot j}\Sigma_i a_i\pi_{i\cdot}}\cdot\pi_{ij}=\frac{p_{i\cdot}p_{\cdot j}}{(\Sigma_j b_j\pi_{\cdot j})(\Sigma_i a_i\pi_{i\cdot})}=p_{i\cdot}p_{\cdot j} \tag{2.6}$$

since $\Sigma_{ij}a_i b_j\pi_{ij}=1$.

The hypothesis to be tested is then the independence of the two classifications subject to the restraints $np_{i\cdot}=x_{i\cdot}$ and $np_{\cdot j}=x_{\cdot j}$, the fixed marginal totals.

Theorem 2.1 is stated in terms of a two-way contingency table for notational convenience. For a three-way contingency table, if $\pi_{ijk}=\pi_{i\cdot\cdot}\pi_{\cdot j\cdot}\pi_{\cdot\cdot k}$, then $p^*_{ijk}=a_i b_j c_k \pi_{ijk}$ and the hypothesis to be

tested is $p_{ijk}=p_{i..}p_{.j.}p_{..k}$, following the same derivation as the two-way table exactly. We shall define all such hypotheses where the one-way marginals are completely specified as the no first-order interaction hypothesis.

Extending this concept, we shall define no second-order interaction in a three-way contingency table as represented by the p^*_{ijk} distribution when all the two-way marginals are considered as fixed and for appropriate selection of π_{ijk}. The justification for this formulation will be discussed in subsection 3.2. Theorem 2.1 can be then restated as

THEOREM 2.1A. *Given a contingency table* $\{\pi_{ijk}\}$, $i=1, 2, \ldots, r, j=1, 2, \ldots, c, k=1, 2, \ldots, d, \Sigma_{ijk}\pi_{ijk}=1$, *where the* $\pi_{ijk}>0$ *represent cell probabilities of some reasonable hypothesis. Consider all contingency tables* $\{p_{ijk}\}$ *of the same dimension with fixed two-way marginals* $p_{ij\cdot}$, $p_{\cdot jk}$, *and* $p_{i\cdot k}$, *then the minimum value of the quantity*

$$I(p:\pi)=\Sigma_{ijk}p_{ijk}\ln\frac{p_{ijk}}{\pi_{ijk}}$$

is attained for $p_{ijk}=p^*_{ijk}=a_{ij}b_{jk}c_{ik}\pi_{ijk}$, $\Sigma_{ijk}a_{ij}b_{jk}c_{ik}\pi_{ijk}=1$, *where* a_{ij}, b_{jk}, *and* c_{ik} *are functions of the given two-way marginal probabilities. Equivalently, the condition may be stated as*

$$\ln\frac{p^*_{ijk}}{\pi_{ijk}}=\ln a_{ij}+\ln b_{jk}+\ln c_{ik}, \tag{2.7}$$

representing no second-order interaction among the three classifications.

To compute the numerical values of p^*_{ijk}, we need

THEOREM 2.2. *The set of* p^*_{ij} *in Theorem 2.1 can be computed by an iterative procedure alternatively satisfying one and then the other marginal restraints. The iteration is given by*

$$p^{(2n-1)}_{ij}=\frac{p_{i\cdot}}{p^{(2n-2)}_{i\cdot}}p^{(2n-2)}_{ij}, \qquad p^{(2n)}_{ij}=\frac{p_{\cdot j}}{p^{(2n-1)}_{\cdot j}}p^{(2n-1)}_{ij}, \qquad n=1, 2, \ldots, \qquad p^{(0)}_{ij}=\pi_{ij}.$$

If $p^{(N)}_{ij}$ *represent the value of the cell probabilities after the* N*th iteration, then either* $p^{(N)}_{ij}=f_{ij}=p^*_{ij}$ *for some finite* N, *or* $p^{(\infty)}_{ij}=p^*_{ij}$.

We shall indicate the first few steps of the iteration process for a two-way table using the relationship

$$p^*_{ij}=a_ib_j\pi_{ij}, \qquad p_{i\cdot}=a_i\Sigma_jb_j\pi_{ij}, \qquad p_{\cdot j}=b_j\Sigma_ia_i\pi_{ij}$$

Let $b^{(1)}_j=1$, then

$$p_{i\cdot}=a^{(1)}_i\pi_{i\cdot}, \qquad p^{(1)}_{ij}=\frac{p_{i\cdot}}{\pi_{i\cdot}}\pi_{ij}=a^{(1)}_ib^{(1)}_j\pi_{ij},$$

$$p_{\cdot j}=b^{(2)}_j\Sigma_ia^{(1)}_i\pi_{ij}, \qquad p^{(2)}_{ij}=\frac{p_{\cdot j}}{p^{(1)}_{\cdot j}}p^{(1)}_{ij}=a^{(1)}_ib^{(2)}_j\pi_{ij},$$

$$p_{i\cdot}=a^{(2)}_i\Sigma_jb^{(2)}_j\pi_{ij}, \qquad p^{(3)}_{ij}=\frac{p_{i\cdot}}{p^{(2)}_{i\cdot}}p^{(2)}_{ij}=a^{(2)}_ib^{(2)}_j\pi_{ij},$$

$$p_{\cdot j}=b^{(3)}_j\Sigma_ia^{(2)}_i\pi_{ij}, \qquad p^{(4)}_{ij}=\frac{p_{\cdot j}}{p^{(3)}_{\cdot j}}p^{(3)}_{ij}=a^{(2)}_ib^{(3)}_j\pi_{ij}.$$

. . . . . .

$$p_{i\cdot} = a_i^{(n)} \Sigma_j b_j^{(n)} \pi_{ij} = p_{i\cdot}^{(2n-1)}, \qquad p_{ij}^{(2n-1)} = \frac{p_{i\cdot}}{p_{i\cdot}^{(2n-2)}} p_{ij}^{(2n-2)} = a_i^{(n)} b_j^{(n)} \pi_{ij},$$

$$p_{\cdot j} = b_j^{(n+1)} \Sigma_i a_i^{(n)} \pi_{ij} = p_{\cdot j}^{(2n)}, \qquad p_{ij}^{(2n)} = \frac{p_{\cdot j}}{p_{\cdot j}^{(2n-1)}} p_{ij}^{(2n-1)} = a_i^{(n)} b_j^{(n+1)} \pi_{ij},$$

etc.

Of course if $\pi_{ij} = \pi_{i\cdot}\pi_{\cdot j}$, then after one cycle of iteration on the two marginals, we have

$$p_{ij}^{(2)} = \frac{p_{\cdot j}}{p_{\cdot j}^{(1)}} p_{ij}^{(1)} = \frac{p_{\cdot j}}{\Sigma_i \frac{p_{i\cdot}}{\pi_{i\cdot}} \pi_{i\cdot}\pi_{\cdot j}} \cdot \frac{p_{i\cdot}}{\pi_{i\cdot}} \pi_{i\cdot}\pi_{\cdot j}$$

$$= \frac{p_{\cdot j}}{\pi_{\cdot j}} \cdot p_{i\cdot}\pi_{\cdot j}$$

$$= p_{i\cdot}p_{\cdot j}$$

and the marginal restraints are satisfied exactly. Hence the iteration process terminates and the solution is exact.

The results of iteration with different sets of specified marginals for a four-way contingency table π_{ijkl}, $i = 1, \ldots, r$, $j = 1, \ldots, c$, $k = 1, \ldots, d$, and $l = 1, \ldots, t$, are given below for purpose of illustration.

Let the given marginals be

(2.8) $$p_{i\ldots}, \qquad p_{\cdot j\cdot\cdot}, \qquad p_{\cdot\cdot k\cdot}, \qquad p_{\cdot\cdot\cdot l}$$

then

(2.9)
$$p_{ijkl}^{*} = a_i b_j c_k d_l \pi_{ijkl}$$

$$p_{i\ldots} = a_i \Sigma_{jkl} b_j c_k d_l \pi_{ijkl}$$

$$p_{\cdot j\cdot\cdot} = b_j \Sigma_{ikl} a_i c_k d_l \pi_{ijkl}$$

$$p_{\cdot\cdot k\cdot} = c_k \Sigma_{ijl} a_i b_j d_l \pi_{ijkl}$$

$$p_{\cdot\cdot\cdot l} = d_l \Sigma_{ijk} a_i b_j c_k \pi_{ijkl}$$

The iterative solution of the system (2.9) cycles through

(2.10)
$$p_{ijkl}^{(4n+1)} = \frac{p_{i\ldots}}{p_{i\ldots}^{(4n)}} p_{ijkl}^{(4n)}, \qquad p_{ijkl}^{(4n+2)} = \frac{p_{\cdot j\cdot\cdot}}{p_{\cdot j\cdot\cdot}^{(4n+1)}} p_{ijkl}^{(4n+1)},$$

$$p_{ijkl}^{(4n+3)} = \frac{p_{\cdot\cdot k\cdot}}{p_{\cdot\cdot k\cdot}^{(4n+2)}} p_{ijkl}^{(4n+2)}, \qquad p_{ijkl}^{(4n+4)} = \frac{p_{\cdot\cdot\cdot l}}{p_{\cdot\cdot\cdot l}^{(4n+3)}} p_{ijkl}^{(4n+3)}.$$

Let the given marginals be

(2.11) $$p_{i\ldots}, \qquad p_{\cdot j\cdot\cdot} \qquad \text{and } p_{\cdot\cdot kl}.$$

Then the problem is essentially that of a three-way table p_{ijm} where $m=(k, l)=1, \ldots, dt$. Since given $p_{..kl}$ determines the marginals $p_{..k.}$ and $p_{...l}$, that is (2.11)$\Rightarrow$(2.8),

$$\Sigma_{ijkl} p^*_{ijkl} \ln \frac{p^*_{ijkl}}{\pi_{ijkl}} \leq \Sigma_{ijm} p^*_{ijm} \ln \frac{p^*_{ijm}}{\pi_{ijm}}.$$

Let the given marginals be

(2.12) $$p_{ij..}, \quad p_{i.k.}, \quad p_{i..l}, \quad p_{.jk.}, \quad p_{.j.l}, \quad p_{..kl},$$

then

(2.13)
$$p^*_{ijkl} = a_{ij} b_{ik} c_{il} d_{jk} e_{jl} f_{kl} \pi_{ijkl},$$

$$p_{ij..} = a_{ij} \Sigma_{kl} b_{ik} c_{il} d_{jk} e_{jl} f_{kl} \pi_{ijkl},$$

$$\ldots\ldots\ldots\ldots\ldots$$

$$p_{..kl} = f_{kl} \Sigma_{ij} a_{ij} b_{ik} c_{il} d_{jk} e_{jl} \pi_{ijkl},$$

and the iterative solution of the system (2.13) cycles through

(2.14) $$p^{(6n+1)}_{ijkl} = \frac{p_{ij..}}{p^{(6n)}_{ij..}} p^{(6n)}_{ijkl}, \ \ldots, \ p^{(6n+6)}_{ijkl} = \frac{p_{..kl}}{p^{(6n+5)}_{..kl}} p^{(6n+5)}_{ijkl}.$$

Since the marginals given in (2.12) determine those given in (2.8) and (2.11), i.e.,

(2.12) $\Rightarrow$ (2.11) $\Rightarrow$ (2.8), it follows that

(2.15) $$I(p^* : \pi | 2.8) \leq I(p^* : \pi | 2.11) \leq I(p^* : \pi | 2.12).$$

If the given marginals are

(2.16) $$p_{ijk.}, \quad p_{ij.l}, \quad p_{i.kl} \text{ and } p_{.jkl},$$

then

(2.17)
$$p^*_{ijkl} = a_{ijk} b_{ijl} c_{ikl} d_{jkl} \pi_{ijkl},$$

$$p_{ijk.} = a_{ijk} \Sigma_l b_{ijl} c_{ikl} d_{jkl} \pi_{ijkl},$$

$$\ldots\ldots\ldots\ldots\ldots$$

$$p_{.jkl} = d_{jkl} \Sigma_i a_{ijk} b_{ijl} c_{ikl} \pi_{ijkl},$$

and the iterative solution of the system (2.17) cycles through

$$p^{(4n+1)}_{ijkl} = \frac{p_{ijk.}}{p^{(4n)}_{ijk.}} p^{(4n)}_{ijkl}, \ \ldots, \ p^{(4n+4)}_{ijkl} = \frac{p_{.jkl}}{p^{(4n+3)}_{.jkl}} p^{(4n+3)}_{ijkl}.$$

Since (2.16) $\Rightarrow$ (2.12) $\Rightarrow$ (2.11) $\Rightarrow$ (2.8), it follows that

(2.18) $$I(p^* : \pi | 2.8) \leq I(p^* : \pi | 2.11) \leq I(p^* : \pi | 2.12) \leq I(p^* : \pi | 2.16).$$

These relationships will be useful in the construction of analysis of information tables to be described in subsections 3.1 and 3.2. The appropriate choice of π_{ijkl} will also be deferred for later discussion.

A third result we shall need is

THEOREM 2.3 *The equality*

$$I(p : \pi) = I(p : p^*) + I(p^* : \pi) \tag{2.19}$$

holds true for p* *computed by the procedure stated in Theorem 2.2 where the* p*- *and* p*-distribution have common specified marginals.*

This is a special case of a property of the minimum discrimination information and can be deduced from a theorem in Kullback and Khairat [1966]. We demonstrate the theorem as applied to a three-way contingency table when all two-way marginals are considered fixed, and where

$$\Sigma_k p^*_{ijk} = \Sigma_k p_{ijk} = p_{ij\cdot},$$

$$\Sigma_j p^*_{ijk} = \Sigma_j p_{ijk} = p_{i\cdot k},$$

$$\Sigma_i p^*_{ijk} = \Sigma_i p_{ijk} = p_{\cdot jk}.$$

We have

$$\Sigma_{ijk} p^*_{ijk} \ln \frac{p^*_{ijk}}{\pi_{ijk}} \tag{2.20}$$

$$= \Sigma_{ijk} p^*_{ijk} \ln a_{ij} + \Sigma_{ijk} p^*_{ijk} \ln b_{jk} + \Sigma_{ijk} p^*_{ijk} \ln c_{ik}$$

$$= \Sigma_{ij} p_{ij\cdot} \ln a_{ij} + \Sigma_{jk} p_{\cdot jk} \ln b_{jk} + \Sigma_{ik} p_{i\cdot k} \ln c_{ik}$$

$$= \Sigma_{ijk} p_{ijk} \ln \frac{p^*_{ijk}}{\pi_{ijk}}.$$

Hence,

$$I(p : \pi) = \Sigma_{ijk} p_{ijk} \ln \frac{p_{ijk}}{\pi_{ijk}}$$

$$= \Sigma_{ijk} p_{ijk} \ln \frac{p_{ijk}}{p^*_{ijk}} + \Sigma_{ijk} p_{ijk} \ln \frac{p^*_{ijk}}{\pi_{ijk}}$$

$$= I(p : p^*) + I(p^* : \pi).$$

2.3. The No-Interaction Hypothesis as a Form of "Generalized Independence"

The formulation of no second-order interaction given in theorem 2.1A suggests that all no interaction hypotheses can be defined in a similar manner, depending on the marginals which are considered given and fixed. Since higher-order marginals determine all lower-order marginals, it is natural to consider the π-distribution as the uniform distribution, corresponding to the case where no marginals are specified, as a general form of independence. For the uniform distribution, $p^*_{ijkl} = \pi_{ijkl} = \dfrac{1}{rcdt}$ in a four-way contingency table. Given all one-way marginals and taking π_{ijkl}

$= \frac{1}{rcdt}$, we obtain

$$p^*_{ijkl} = p_{i\cdots} p_{\cdot j\cdot\cdot} p_{\cdot\cdot k\cdot} p_{\cdot\cdot\cdot l} \tag{2.21}$$

i.e., the distribution which "most resembles" the uniform distribution subject to the four one-way marginal restraints. Derivation of (2.21) follows exactly as that of (2.6). Given all two-way marginals, the distribution that "most resembles" the uniform distribution subject to the six two-way marginals restraints is the p^*_2 distribution representing no second-order interaction. Given all four three-way marginals, we obtain p^*_3 corresponding to no third-order interaction.

In this sense the no-interaction hypotheses can be considered as generalized forms of independence hypotheses, where the "degrees" of independence that can be realized depend on the marginal restraints imposed. Each time we add on a restraint, we obtain a p^* distribution corresponding to the condition of minimum discrimination information subject to the additional restraints, and corresponding to the appropriate null hypothesis to be tested given this additional restraint.

Hence we may state the principle of minimum discrimination information for the generation of appropriate hypotheses:

"If certain marginal probabilities of a contingency table are considered given or fixed, then the appropriate interaction hypothesis to be tested, subject to these fixed marginal restraints, is the hypothesis represented by the unique set of cell probabilities p^*_{ijkl} satisfying these restraints and yielding the minimum value of discrimination information

$$I(p : \pi) = \Sigma_{ijkl} p_{ijkl} \ln p_{ijkl} + \ln rcdt \tag{2.22}$$

for all p_{ijkl}."

It can be shown that all the usual "classical" hypotheses can be generated by the application of this principle. If complete sets of marginals are considered given in a four-way table, we arrive at the following sequence.

Marginals considered as fixed							No-interaction hypothesis
$p_{\cdots\cdot} = 1$						$p^*_0 = \frac{1}{rcdt}$	zeroth-order (uniform).
$p_{i\cdots\cdot}$	$p_{\cdot j\cdot\cdot\cdot}$	$p_{\cdot\cdot k\cdot\cdot}$	$p_{\cdot\cdot\cdot l}$			p^*_1	first-order (4-way independence).
$p_{ij\cdot\cdot\cdot}$	$p_{i\cdot k\cdot\cdot}$	$p_{i\cdot\cdot l\cdot}$	$p_{\cdot jk\cdot\cdot}$	$p_{\cdot j\cdot l\cdot}$	$p_{\cdot\cdot kl}$	p^*_2	second-order.
$p_{ijk\cdot\cdot}$	$p_{ij\cdot l\cdot}$	$p_{i\cdot kl\cdot}$	$p_{\cdot jkl}$			p^*_3	third-order.
p_{ijkl}						$p^*_4 = p_{ijkl}$	fourth-order (no test).

If only part of a complete set of marginals are given, a conditional type of independence is generated. Some of these hypotheses for which the p^*_{ijkl} can be explicitly expressed in terms of the marginals are given in table 2.1. We demonstrate here the generation of the conditional inde-

pendence in a three-way table when two of the two-way marginals, $p_{ij\cdot}$ and $p_{\cdot jk}$ are assumed to be fixed.

TABLE 2.1. *Some explicit expressions for* p^*_{ijkl}

Marginal restraints	p^*_{ijkl}
$p\ldots\ldots = 1$	$1/rcdt$
$p_{i\ldots}$	$p_{i\ldots}/cdt$
$p_{i\ldots}$, $p_{\cdot j\cdot\cdot}$	$p_{i\ldots}p_{\cdot j\cdot\cdot}/dt$
$p_{i\ldots}$, $p_{\cdot j\cdot\cdot}$, $p_{\cdot\cdot k\cdot}$	$p_{i\ldots}p_{\cdot j\cdot\cdot}p_{\cdot\cdot k\cdot}/t$
$p_{i\ldots}$, $p_{\cdot j\cdot\cdot}$, $p_{\cdot\cdot k\cdot}$, $p_{\ldots l}$	$p_{i\ldots}p_{\cdot j\cdot\cdot}p_{\cdot\cdot k\cdot}p_{\ldots l}$
$p_{ij\cdot\cdot}$	$p_{ij\cdot\cdot}/dt$
$p_{ij\cdot\cdot}$, $p_{\cdot\cdot kl}$	$p_{ij\cdot\cdot}p_{\cdot\cdot kl}$
$p_{\cdot j\cdot\cdot}$, $p_{i\cdot\cdot l}$, $p_{\cdot\cdot kl}$	$p_{\cdot j\cdot\cdot}p_{i\cdot\cdot l}p_{\cdot\cdot kl}/p_{\ldots l}$
$p_{ij\cdot\cdot}$, $p_{i\cdot k\cdot}$, $p_{i\cdot\cdot l}$	$p_{ij\cdot\cdot}p_{i\cdot k\cdot}p_{i\cdot\cdot l}/(p_{i\ldots})^2$
$p_{ij\cdot\cdot}$, $p_{i\cdot\cdot l}$, $p_{\cdot\cdot kl}$	$p_{ij\cdot\cdot}p_{i\cdot\cdot l}p_{\cdot\cdot kl}/p_{i\ldots}p_{\ldots l}$
$p_{ij\cdot\cdot}$, $p_{i\cdot\cdot l}$, $p_{\cdot jk\cdot}$	no explicit expression

By theorem 2.1A we have

$$p^*_{ijk} = a_{ij}b_{jk}\pi_{ijk},$$

subject to the restraints

$$\Sigma_i p^*_{ijk} = b_{jk}\Sigma_i a_{ij}\pi_{ijk} = p_{\cdot jk},$$

$$\Sigma_k p^*_{ijk} = a_{ij}\Sigma_k b_{jk}\pi_{ijk} = p_{ij\cdot}.$$

Hence

$$p^*_{ijk} = \frac{p_{\cdot jk}}{(\Sigma_i a_{ij}\pi_{ijk})} \cdot \frac{p_{ij\cdot}}{(\Sigma_k b_{jk}\pi_{ijk})} \cdot \pi_{ijk}. \tag{2.23}$$

If we let $\pi_{ijk} = \dfrac{1}{rcd}$, then

$$p^*_{ijk} = \frac{p_{\cdot jk}p_{ij\cdot}}{\Sigma_{ik}a_{ij}b_{jk}\pi_{ijk}} = \frac{p_{\cdot jk}p_{ij\cdot}}{p_{\cdot j\cdot}}, \tag{2.24}$$

or the conditional independence hypothesis of the row and depth classification given the column classification.

It is of interest to note that the same expression for p^*_{ijk} in (2.24) is obtained whether we use

$$\pi_{ijk} = 1/rcd \tag{2.25}$$

$$\pi_{ijk} = \pi_{i..}\pi_{.j.}\pi_{..k}, \text{ or}$$

$$\pi_{ijk} = \pi_{ij.}\pi_{.jk}/\pi_{.j.}.$$

Thus, as long as π_{ijk} represent the condition of generalized independence corresponding to marginal restraints of an order lower or equal to the given marginal restraints, the same set of p^*_{ijk} will be generated by our procedure. In the present case

given $\qquad (p_{ij.}, p_{.jk}) \Rightarrow (p_{i..}, p_{.j.}, p_{..k}) \Rightarrow p_{...}$.

A simple proof of this property is as follows. The set of p^*_{ijk} is obtained by minimizing the discrimination information

$$I(p:\pi) = \Sigma_{ijk} p_{ijk} \ln \frac{p_{ijk}}{\pi_{ijk}}$$

subject to given marginal restraints. Now

$$I(p:\pi) = \Sigma_{ijk} p_{ijk} \ln p_{ijk} - \Sigma_{ijk} p_{ijk} \ln \pi_{ijk} \tag{2.26}$$

and the second term of the expression in the right-hand side of (2.26) reduces to a constant no matter which form of π_{ijk} in (2.25) is used. Hence the same p^*_{ijk} will give the minimum value of (2.26). Good [1966] showed that the chains of hypotheses generated by the principle of minimum discriminability depend only on the increasing sequence of linear constraints, irrespective of which of the existing hypotheses the new ones are referred to.

2.4. Consistency of Information-Theoretic Definition of No Second-Order Interaction With Other Formulations

We shall show that the definition of no second-order interaction given in Theorem 2.1A is consistent with the formulations given by Bartlett, and Roy and Kastenbaum represented by (1.1) and (1.2). We may remark here also that the p^*-distribution satisfies all the four requirements in subsection 1.4. The p^*-distribution satisfies the requirements of (a) fixed marginal totals (b) symmetry and (c) unique set of cell probabilities because of the way it is derived. Additivity is a property of m.d.i.s. [Theorem 2.1, ch. 2, Kullback 1959] which facilitates the construction of analysis of information tables.

For an $r \times c$ table with given set of cell probabilities p_{ij} and π_{ij}, let us find the table with the same marginals as p_{ij} but minimizing the expression

$$f(d_{ij}) = \Sigma_{ij}(p_{ij} + d_{ij}) \ln \frac{(p_{ij} + d_{ij})}{\pi_{ij}}$$

with

$$\Sigma_i d_{ij} = \Sigma_j d_{ij} = 0.$$

Since $f(d_{ij})$ is a convex function, its minimum is given by the d_{ij}'s satisfying the set of equations

$$\frac{\partial f(d_{ij})}{\partial d_{ij}} = 0 = \ln \frac{p_{ij}+d_{ij}}{\pi_{ij}} - \ln \frac{p_{ic}+d_{ic}}{\pi_{ic}} - \ln \frac{p_{rj}+d_{rj}}{\pi_{rj}} + \ln \frac{p_{rc}+d_{rc}}{\pi_{rc}}.$$

For the values of d_{ij}'s satisfying the above let $p_{ij}+d_{ij}=p^*_{ij}$, then the set of equations reduces to

$$\frac{p^*_{ij}}{\pi_{ij}} \cdot \frac{p^*_{rc}}{\pi_{rc}} = \frac{p^*_{ic}}{\pi_{ic}} \cdot \frac{p^*_{rj}}{\pi_{rj}}, \tag{2.27}$$

and all are satisfied by

$$p^*_{ij} = a_i b_j \pi_{ij}.$$

This procedure is essentially what Bartlett used in getting a solution to the no second-order interaction hypothesis in a $2\times2\times2$ table. Bartlett specified the condition of no second-order interaction to be

$$\frac{p_{111}p_{122}}{p_{112}p_{121}} = \frac{p_{211}p_{222}}{p_{212}p_{221}}. \tag{2.28}$$

For observed cell frequencies x_{ijk}, he solved for Δ in the equation

$$\frac{(x_{111}+\Delta)(x_{122}+\Delta)}{(x_{112}-\Delta)(x_{121}-\Delta)} = \frac{(x_{211}-\Delta)(x_{222}-\Delta)}{(x_{212}+\Delta)(x_{221}+\Delta)}, \tag{2.29}$$

and computed

$$X^2 = \Delta^2 \Sigma_{ijk} \frac{1}{x_{ijk}}.$$

In fact, Bartlett's X^2 is an approximation to $2n\hat{I}$ given in (3.3). If we let $x_{ijk}=x^*_{ijk}\pm\Delta$ and expand $x_{ijk}\ln x_{ijk}$ about $x^*_{ijk}\ln x^*_{ijk}$ by a Taylor series expansion up to Δ^2, we have

$$x_{ijk}\ln x_{ijk} \doteq x^*_{ijk}\ln x^*_{ijk} \pm \Delta(\ln x^*_{ijk}+1) + \frac{\Delta^2}{2}\left(\frac{1}{x^*_{ijk}}\right).$$

Summing over $i, j, k=1, 2$,

$$\Sigma_{ijk}x_{ijk}\ln x_{ijk} \doteq \Sigma_{ijk}x^*_{ijk}\ln x^*_{ijk} + \Sigma_{ijk}(\pm\Delta)(\ln x^*_{ijk}+1) + \frac{\Delta^2}{2}\Sigma_{ijk}\frac{1}{x^*_{ijk}}.$$

Since the middle term on the right hand side is equal to zero by (2.28),

$$2n\hat{I} = 2\Sigma_{ijk}x_{ijk}\ln\frac{x_{ijk}}{x^*_{ijk}} \doteq \Delta^2\Sigma_{ijk}\frac{1}{x_{ijk}} = X^2.$$

Also it can be checked readily by substitution that if a π_{ijk} distribution satisfies (2.28), then the p^*_{ijk} distribution also satisfies (2.28) when $p^*_{ijk}=a_ib_jc_k\pi_{ijk}$. The same is true for the set of conditions of no second-order interaction in an $r\times c\times d$ table given by Roy and Kastenbaum in eq (1.2).

It is to be noted also that Good's Principle of Minimal Discriminability is essentially the same as our Principle of Minimum Discrimination Information. Darroch's suggested procedure and our

312-532 O - 68 - 2

procedure also share a number of similarities. However, we have demonstrated that many hypotheses of interest for contingency tables can be generated through one unified procedure based on information theory and the hypothesis of no second-order interaction is no exception. Furthermore, the properties of the minimum discrimination information statistics, convexity and additivity, allow us to derive and interpret these statistics naturally, and to construct the analysis of information tables for an overall comparison between the sample and the nested sequence of hypotheses.

For other related literature dealing with a similar problem but not in the testing of no-interaction hypotheses in contingency tables, we cite P. M. Lewis II [1959] and D. T. Brown [1959]. Lewis, on an ad hoc basis, considered approximations to a discrete probability distribution over the space of binary random variables by distributions which are products of various marginal distributions of the original one and measured the goodness of fit by the discrimination information measure. D. T. Brown extended this notion to using an approximating distribution having certain marginals the same as those of the original distribution. He described an iterative procedure which is the same as the example following theorem 2.2, and showed that the goodness of the approximation improves at each step of the iteration using discrimination information as a measure of goodness. The procedure he described is the special case of an n-way $2\times 2\times \ldots \times 2$ table with initial cell probabilities all equal to $1/2^n$.

3. Analysis of Multidimensional Contingency Tables and the Interpretation of Results

3.1. The m.d.i.s. for the No-Interaction Hypothesis

In the last section we have shown that the no-interaction hypothesis can be considered as a hypothesis of generalized independence, subject to fixed marginal restraints. Furthermore, the unique set of p^*-distributions can be computed by a convergent iterative process alternatively satisfying the given marginals.

Let p_0 represent the cell probabilities under the hypothesis of uniform distribution. We say that $\{p^*\}$ is the table that most resembles $\{p_0\}$ subject to these marginal restraints, or there is no interaction between $\{p^*\}$ and $\{p_0\}$ in the sense that

$$I(p^*:p_0)=\Sigma p^* \ln\frac{p^*}{p_0}$$

is a minimum for all p's consistent with dimension of the table and the given restraints. For any other table we may write

$$\Sigma p \ln\frac{p}{p_0}=\Sigma p^* \ln\frac{p^*}{p_0}+\left\{\Sigma p \ln\frac{p}{p_0}-\Sigma p^* \ln\frac{p^*}{p_0}\right\}. \tag{3.1}$$

Since the first term on the right represents the condition of no interaction, the term in the bracket

$$\Sigma p \ln\frac{p}{p_0}-\Sigma p^* \ln\frac{p^*}{p_0}=\Sigma p \ln\frac{p}{p^*} \tag{3.2}$$

is then a measure of interaction, or the departure of the p-distribution from the no-interaction distribution. The equality in (3.2) follows from theorem 2.3.

Given an observed sample with cell frequencies x_{ijk} in a three-way table, and let $x_{ij.}$, $x_{i.k}$, and $x_{.jk}$ be the given marginal restraints, then the m.d.i.s. for testing the hypothesis of no second-order interaction is

$$2nI(\hat{p}:p^*)=2\Sigma_{ijk}x_{ijk} \ln\frac{x_{ijk}}{x^*_{ijk}} \tag{3.3}$$

where $x^*_{ijk} = np^*_{ijk}$, and $\hat{p} = x_{ijk}/n$.

The distribution of $2nI(\hat{p}:p^*)$ is asymptotically chi-squared as shown in Kullback [1959], Kupperman [1957] with $(r-1)(c-1)(d-1)$ degrees of freedom. The same result is obtained if we note that p^*_{ijk}'s are RBAN estimators in the sense of Neyman [1949] of the cell probabilities under the hypothesis of no second-order interaction, or CAN estimators of Rao [1965, p. 288]. The degrees of freedom are calculated from the general principle of equivalence of degrees of freedom and the number of independent restraints imposed by the specified marginals. In this case the degrees of freedom are

$$rcd-1-(r-1)(c-1)-(r-1)(d-1)-(c-1)(d-1)-(r-1)-(c-1)-(d-1) = (r-1)(c-1)(d-1). \tag{3.4}$$

For a four-way table, the relationship between various interactions corresponding to completely specified sets of marginals are given in table 3.1. The following notations are used in the computation of degrees of freedom:

$$N = rcdt-1 = N_1+N_2+N_3+N_4 \tag{3.5}$$

$$N_1 = (r-1)+(c-1)+(d-1)+(t-1)$$

$$N_2 = (r-1)(c-1)+(r-1)(d-1)+(r-1)(t-1)+(c-1)(d-1)+(c-1)(t-1)+(d-1)(t-1)$$

$$N_3 = (r-1)(c-1)(d-1)+(r-1)(c-1)(t-1)+(r-1)(d-1)(t-1)+(c-1)(d-1)(t-1)$$

$$N_4 = (r-1)(c-1)(d-1)(t-1).$$

TABLE 3.1. *Analysis of information—four-way table*

Information	For testing the hypothesis of	Degrees of freedom
$2nI(\hat{p} : \hat{p}^*_3)$ $2nI(\hat{p}^*_3 : \hat{p}^*_2)$	No third-order interaction	$N-N_1-N_2-N_3=N_4$ N_3
$2nI(\hat{p} : \hat{p}^*_2)$ $2nI(\hat{p}^*_2 : \hat{p}^*_1)$	No second-order interaction	$N-N_1-N_2$ N_2
$2nI(\hat{p} : \hat{p}^*_1)$ $2nI(\hat{p}^*_1 : p_0)$	Independence (No first-order interaction)	$N-N_1$ N_1
$2nI(\hat{p} : p_0)$	Uniformity	N

In table 3.1 we have specified a complete set of marginals as fixed for each hypothesis. This restriction is clearly unnecessary. We shall define the p^*-distribution generated by a partial set

of marginals or a mixed set of marginals of different order as the no "mixed-order interaction" hypothesis. An example of mixed-order interaction is the conditional independence hypothesis given by (2.24), where only two of the two-way marginals are specified in a three-way table.

To simplify the notation for a step by step analysis of a four-way table, let us denote the quantity

$$-\Sigma_{ijkl} p^*_{ijkl} \ln p^*_{ijkl}$$

by $H(\ )$ where the indices within the bracket stand for the marginals that are considered fixed. If all the two-way marginals are considered fixed, we may write H (given two-way), or other descriptive phrases with defined meanings. The symbol $\hat{I}(\ )$ will be used to denote the difference between $H(\ )$ and H (data).

We note that the "H" notation used here is the notation for entropy. For the case $\pi_{ijkl} = 1/rcdt$, the problem of minimizing $I(p:\pi)$ in (2.4) subject to certain restraints is equivalent to minimizing

$$\Sigma_{ijkl} p_{ijkl} \ln p_{ijkl} + \ln rcdt, \tag{3.6}$$

or maximizing the entropy

$$-\Sigma_{ijkl} p_{ijkl} \ln p_{ijkl} \tag{3.7}$$

subject to the same restraints. The latter problem has been considered by Good [1963, 1965, 1966].

Since higher-order marginals determine all lower marginals, we have, corresponding to (2.18), the following:

$$\begin{aligned} H \text{ (data)} &\leqslant H \text{ (given 3-way)} = H_3 \\ &\leqslant H \text{ (given 2-way)} = H_2 \\ &\leqslant H \text{ (given 1-way)} = H_1 \\ &\leqslant H \text{ (uniform)} \quad = H_0 = \ln rcdt. \end{aligned} \tag{3.8}$$

Hence,

$$\begin{aligned} \hat{I} \text{ (given 1-way)} &= H_1 - H \text{ (data)} \\ &= [H_2 - H \text{ (data)}] + (H_1 - H_2) \\ &\geqslant \hat{I} \text{ (given 2-way)} \end{aligned} \tag{3.9}$$

$$\begin{aligned} \hat{I} \text{ (given 2-way)} &= H_2 - H \text{ (data)} \\ &= [H_3 - H \text{ (data)}] + (H_2 - H_3) \\ &\geqslant \hat{I} \text{ (given 3-way)} \geqslant 0. \end{aligned} \tag{3.10}$$

In table 3.2 the two-way marginals are added one by one to the four one-way marginals until all six are specified; then the three-way marginals are added one by one to the complete set of two-way marginals until all four are specified. The components of information are expressed in terms of the differences in entropies, and when possible, also in terms of the form that can be obtained through the convexity property of m.d.i.s.

TABLE 3.2. *Interactions in a four-way table*

Marginal restraints added	p^*_{ijkl}	Information	Form obtained by convexity property	d.f.
$p_{i\cdots}, p_{\cdot j\cdot\cdot}, p_{\cdot\cdot k\cdot}, p_{\cdot\cdot\cdot l}$	$p_{i\cdots}p_{\cdot j\cdot\cdot}p_{\cdot\cdot k\cdot}p_{\cdot\cdot\cdot l}$	$H(i,j,k,l)-H(\text{data})$	$\Sigma_{ijkl}\hat{p}_{ijkl}\ln\dfrac{\hat{p}_{ijkl}}{p_{i\cdots}p_{\cdot j\cdot\cdot}p_{\cdot\cdot k\cdot}p_{\cdot\cdot\cdot l}}$	$rcdt-1-(r-1)-(c-1)$ $-(d-1)-(t-1)=N-N_1$
$p_{\cdot\cdot kl}$	$p_{i\cdots}p_{\cdot j\cdot\cdot}p_{\cdot\cdot kl}$	$H(i,j,k,l)-H(i,j,kl)$ $=H(k,l)-H(kl)$ $H(i,j,kl)-H(\text{data})$	$\Sigma_{kl}\hat{p}_{\cdot\cdot kl}\ln\dfrac{\hat{p}_{\cdot\cdot kl}}{p_{\cdot\cdot k\cdot}p_{\cdot\cdot\cdot l}}$ $\Sigma_{ijkl}\hat{p}_{ijkl}\ln\dfrac{\hat{p}_{ijkl}}{p_{i\cdots}p_{\cdot j\cdot\cdot}p_{\cdot\cdot kl}}$	$(d-1)(t-1)$ $N-N_1-(d-1)(t-1)$
$p_{i\cdot\cdot l}$	$p_{\cdot j\cdot\cdot}\dfrac{p_{i\cdot\cdot l}p_{\cdot\cdot kl}}{p_{\cdot\cdot\cdot l}}$	$H(i,j,kl)-H(j,kl,il)$ $=H(i,l)-H(il)$ $H(j,kl,il)-H(\text{data})$	$\Sigma_{il}\hat{p}_{i\cdot\cdot l}\ln\dfrac{\hat{p}_{i\cdot\cdot l}}{p_{i\cdots}p_{\cdot\cdot\cdot l}}$ $\Sigma_{ijkl}\hat{p}_{ijkl}\ln\dfrac{\hat{p}_{ijkl}}{p_{\cdot j\cdot\cdot}(p_{\cdot\cdot kl}p_{i\cdot\cdot l}/p_{\cdot\cdot\cdot l})}$	$(r-1)(t-1)$ $N-N_1-(d-1)(t-1)$ $-(r-1)(t-1)$
$p_{ij\cdot\cdot}$	$\dfrac{p_{ij\cdot\cdot}p_{\cdot\cdot kl}p_{i\cdot\cdot l}}{p_{k\cdots}p_{\cdot\cdot\cdot l}}$	$H(j,kl,il)-H(kl,il,ij)$ $=H(i,j)-H(ij)$ $H(kl,il,ij)-H(\text{data})$	$\Sigma_{ij}\hat{p}_{ij\cdot\cdot}\ln\dfrac{\hat{p}_{ij\cdot\cdot}}{p_{i\cdots}p_{\cdot j\cdot\cdot}}$ $\Sigma_{ijkl}\hat{p}_{ijkl}\ln\dfrac{\hat{p}_{ijkl}}{\dfrac{p_{ij\cdot\cdot}p_{\cdot\cdot kl}p_{i\cdot\cdot l}}{p_{i\cdots}p_{\cdot\cdot\cdot l}}}$	$(r-1)(c-1)$ $N-N_1-(d-1)(t-1)$ $-(r-1)(t-1)$ $-(r-1)(c-1)$
$p_{\cdot jk\cdot}$		$H(kl,il,ij)-H(kl,il,ij,jk)$ $H(kl,il,ij,jk)-H(\text{data})$	$\Sigma_{jk}\hat{p}_{\cdot jk\cdot}\ln\dfrac{\hat{p}_{\cdot jk\cdot}}{\Sigma_{il}\dfrac{p_{ij\cdot\cdot}p_{\cdot\cdot kl}p_{i\cdot\cdot l}}{p_{i\cdots}p_{\cdot\cdot\cdot l}}}$	$(c-1)(d-1)$ $N-N_1-(d-1)(t-1)$ $-(r-1)(t-1)$ $-(r-1)(c-1)$ $-(c-1)(d-1)$

TABLE 3.2. *Interactions in a four-way table* – Continued

Marginal restraints added	p^*_{ijkl}	Information	Form obtained by convexity property	d.f.
$p_{i\cdot k\cdot}$		$H(kl, il, ij, jk) - H(kl, il, ij, jk, ik)$ $H(kl, il, ij, jk, ik) - H(\text{data})$	Iteration on indicated two-way marginals	$(r-1)(d-1)$ $N - N_1 - (d-1)(t-1) - (r-1)(t-1) - (r-1)(c-1) - (c-1)(t-1) - (r-1)(d-1)$
$p_{\cdot j\cdot l}$	Second-order interaction	$H(kl, il, ij, jk, ik) - H(\text{given two-way})$ $H(kl, il, ij, jk, ik, jl) - H(\text{data})$		$(c-1)(t-1)$ $N - N_1 - N_2$
Six two-way marginals		$H(\text{given two-way}) - H(\text{data})$		$N - N_1 - N_2$
$p_{ijk\cdot}$		$H(\text{given two-way}) - H(il, jl, kl, ijk)$ $H(il, jl, kl, ijk) - H(\text{data})$		$(r-1)(c-1)(d-1)$ difference
$p_{ij\cdot l}$		$H(il, jl, kl, ijk) - H(ijk, ijl)$ $H(ijk, ijl) - H(\text{data})$		$(r-1)(c-1)(t-1)$ difference
$p_{i\cdot kl}$		$H(ijk, ijl,) - H(ijk, ijl, ikl)$ $H(ijk, ijl, ikl) - H(\text{data})$		$(r-1)(d-1)(t-1)$ difference
$p_{\cdot jkl}$	Third-order interaction	$H(ijk, ijl, ikl) - H(\text{given three-way})$ $H(\text{given three-way}) - H(\text{data})$		$(c-1)(d-1)(t-1)$ $N - N_1 - N_2 - N_3 = (r-1)(c-1)(d-1)(t-1) = N_4$

We note in table 3.2 that the addition of each two-way marginal restraint generates a hypothesis of two-way independence of the corresponding marginal table, or the conditional two-way independence given one or more marginals. Beginning with the fourth marginal restraint, however, these hypotheses can no longer be expressed in an explicit closed form and the respective p^*-distributions will have to be generated by the iteration procedure.

3.2. Some Typical Second-Order No-Interaction Hypotheses

In many practical applications, the hypothesis of interest is usually suggested by the physical relationship involved in the problem, and the result of the test admits natural interpretations. The no second-order interaction in a three-way table originated in this manner, i.e., it is a test of the sameness of the measure of association between R and C classifications over categories of D [Simpson 1951].

With the addition of another dimension in a four-way table, there are a number of mixed second-order interactions to which there are no corresponding ones in a three-way table. Some of the typical ones are described below.

The interaction of a one-way by two-way interaction over the fourth classification is a mixed second-order interaction. There are six such second-order interactions, corresponding to the six three-way tables with different marginal probabilities, and possibly different dimensions, that can be constructed from a four-way table. Since symmetry is a property of our procedure, these interactions could also be considered as the interaction of one-way by one-way interaction over categories of the two remaining classifications. For example, the second-order interaction $(DT \times R)(C)$ is the same as the second-order interaction $(R \times C)(DT)$.

The analysis of information table for these second-order interactions is given in table 3.3, using the convexity property of the m.d.i.s. to indicate:

(1) how this second-order interaction can be derived, and

(2) the particular marginals which must be specified for the iteration procedure, viz., $p_{ij\cdot\cdot}$, $p_{\cdot jkl}$, and $p_{i\cdot kl}$ in this case.

We note that if we consider

$$p^{(0)}_{ijkl} = \frac{p_{ij\cdot\cdot}\, p_{\cdot jkl}}{p_{\cdot j\cdot\cdot}},$$

then

$$p^{(1)}_{ijkl} = \frac{p_{i\cdot kl}}{p^{(0)}_{i\cdot kl}}\, p^{(0)}_{ijkl}$$

$$= \frac{p_{ij\cdot\cdot}\, p_{\cdot jkl}}{p_{\cdot j\cdot\cdot}} \cdot \frac{p_{i\cdot kl}}{\sum_j \frac{p_{ij\cdot\cdot}\, p_{\cdot jkl}}{p_{\cdot j\cdot\cdot}}},$$

which is exactly the denominator appearing in the expression for second-order interaction. Hence the convexity property of the m.d.i.s. is useful in giving an explicit expression for the p^*_{ijkl} value after the first iteration. This agreement is not surprising since we are utilizing two distinct but consistent properties of the m.d.i.s.

Viewing the four-way table in another perspective, there are four distinct second-order interactions defined as the interaction of the three-way interaction over the fourth classification. The analysis for $(R \times D \times T)(C)$ is shown in table 3.4. The marginals to be considered as specified are

$$p_{ij\cdot\cdot},\ p_{\cdot jk\cdot},\ p_{\cdot j\cdot l},\ \text{and}\ p_{i\cdot kl}.$$

TABLE 3.3. *Mixed-order interactions in a four-way table*

Component due to	Information	d.f.
$(DT\times R)(C)$ Second-order interaction [a]	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{\dfrac{p_{ij\cdot\cdot}p_{\cdot jkl}}{p_{\cdot j\cdot\cdot}}\cdot\dfrac{p_{i\cdot kl}}{\Sigma_j\dfrac{p_{ij\cdot\cdot}p_{\cdot jkl}}{p_{\cdot j\cdot\cdot}}}}$	$(c-1)(r-1)(dt-1)$
$(DT, R)(C)$ Three-way marginals interaction with column	$2\Sigma_{ikl}p_{i\cdot kl}\ln\dfrac{p_{i\cdot kl}}{\Sigma_j\dfrac{p_{ij\cdot\cdot}p_{\cdot jkl}}{p_{\cdot j\cdot\cdot}}}$	$(r-1)(dt-1)$
$DT\times R\|C$ Two-way by one-way interaction, given column	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{p_{ij\cdot\cdot}p_{\cdot jkl}/p_{\cdot j\cdot\cdot}}$	$c(r-1)(dt-1)$

[a] Form shown is the second-order interaction after first iteration.

Conceptually a third-order interaction in a four-way table may be defined as the interaction of the second-order interactions of the three classifications over categories of the fourth classification. The analysis following this line of thought is given in table 3.5, showing the marginals to be specified are

$$p_{ijk\cdot},\ p_{i\cdot kl},\ p_{ij\cdot l},\ \text{and}\ p_{\cdot jkl}.$$

It is clear that we do not have a direct counterpart of third-order interaction in the classical hypotheses. The interpretation of no third-order interaction also becomes obscure in the conventional sense. We propose, therefore, to consider a hypothesis represented by the p^*-distribution as that of a generalized independence (generalized no interaction, no association) among the classifications with given fixed marginals, and give a unified interpretation in the following subsection.

TABLE 3.4. *Mixed-order interactions in a four-way table*

Component due to	Information	d.f.
$(R\times D\times T)(C)$ Second-order interaction [a]	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{\dfrac{p_{ij\cdot\cdot}p_{\cdot jk\cdot}p_{\cdot j\cdot l}}{(p_{\cdot j\cdot\cdot})^2}\cdot\dfrac{p_{i\cdot kl}}{\Sigma_j\dfrac{p_{ij\cdot\cdot}p_{\cdot jk\cdot}p_{\cdot j\cdot l}}{(p_{\cdot j\cdot\cdot})^2}}}$	$(c-1)(rdt-r-d-t+2)$
$(R, D, T)(C)$ Three-way marginals interaction with column	$2\Sigma_{ikl}p_{i\cdot kl}\ln\dfrac{p_{i\cdot kl}}{\Sigma_j\dfrac{p_{ij\cdot\cdot}p_{\cdot jk\cdot}p_{\cdot j\cdot l}}{(p_{\cdot j\cdot\cdot})^2}}$	$rdt-r-d-t+2$
$R\times D\times T\|C$ Three-way interaction, given column	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{\dfrac{p_{ij\cdot\cdot}p_{\cdot jk\cdot}p_{\cdot j\cdot l}}{(p_{\cdot j\cdot\cdot})^2}}$	$c(rdt-r-d-t+2)$

[a] Form shown is the second-order interaction after the first iteration.

TABLE 3.5. *Third-order interaction derived from the convexity property*

Component due to	Information	d.f.
$(R\times T)(D)(C)$ Third-order interaction	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{\dfrac{p_{i\cdot kl}}{\Sigma_j\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}}\cdot\dfrac{p_{ij\cdot l}}{\Sigma_k\frac{p_{i\cdot kl}}{\Sigma_k\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}}}\cdot\dfrac{\Sigma_k\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}}{p_{\cdot jk\cdot}}}$	$(r-1)(c-1)(d-1)(t-1)$
$(R, D, T)(C)$ Three-way marginals interaction with column	$2\Sigma_{ikl}p_{i\cdot kl}\ln\dfrac{p_{i\cdot kl}}{\Sigma_j\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}\cdot\dfrac{p_{ij\cdot l}}{\Sigma_k\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}}}$	$(r-1)(d-1)(t-1)$
$(R\times T)(D)\|C$ Second-order interaction, given column [a]	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}\dfrac{p_{ij\cdot l}}{\Sigma_k\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}}}$	$c(r-1)(d-1)(t-1)$
$(R, T)(D)\|C$ Two-way marginals interaction with depth, given column	$2\Sigma_{ijl}p_{ij\cdot l}\ln\dfrac{p_{ij\cdot l}}{\Sigma_k\frac{p_{ijk\cdot}p_{\cdot jkl}}{p_{\cdot jk\cdot}}}$	$c(r-1)(t-1)$
$R\times T\|CD$ One-way by one-way interaction, given CD	$2\Sigma_{ijkl}p_{ijkl}\ln\dfrac{p_{ijkl}}{p_{ijk\cdot}p_{\cdot jkl}/p_{\cdot jk\cdot}}$	$cd(r-1)(t-1)$

[a] Form shown is the second-order interaction after first iteration.

3.3. Logarithmic Additivity and a General Interpretation of the No-Interaction Hypothesis

In theorem 2.1A, we give the p^*-distribution for no second-order interaction as

$$\ln\frac{p^*_{ijk}}{\pi_{ijk}}=\ln a_{ij}+\ln b_{jk}+\ln c_{ik} \tag{3.11}$$

where a_{ij}, b_{jk} and c_{ik} are functions of the three two-way marginals. In this form, the logarithms of the cell probabilities representing the no second-order interaction hypothesis are seen to be the sum of a constant and the logarithms of contributions from each of the specified marginals. Similarly, for the test of the hypothesis of uniform distribution, we have

$$\ln p^*_{ijk}=\ln\frac{1}{rcd}, \tag{3.12}$$

and for the test of the hypothesis of three-way independence,

$$\ln p^*_{ijk}=\ln\frac{1}{rcd}+\ln a_i+\ln b_j+\ln c_k. \tag{3.13}$$

Hence, if we consider the difference in the logarithms of the cell probabilities between the independence hypothesis and the uniform distribution hypothesis as represented by a row effect, a

column effect, and a depth effect, then the striking similarities between our approach to contingency table analysis and the approach used in analysis of variance become immediately obvious.

To begin with, both analyses deal with multifactor multiresponse data. In the linear hypothesis, an additive model is assumed; in the analysis of contingency tables, a logarithmic additive model is assumed. In both cases the appropriate test statistics can be obtained by minimizing the discrimination information [ch. 10, 11, Kullback 1959]. The residuals in the usual linear analysis represent the difference between the observed values and the values computed from the model using the estimated values of the parameters; the residuals in our analysis represent the differences between the observed cell frequencies and the cell frequencies x^* computed under each particular hypothesis. The main effects and the various interactions in the analysis of variance also find corresponding counterparts in our first-order, second-order, and higher-order interactions. Darroch [1961], Bhakpar [1961], Lindley [1964], and Mantel [1966] have all suggested some analogy between the two types of analyses with a view to simplifying the analysis of multidimensional contingency tables. We remark that the main difference between the two types of analysis is that the marginal restraints requirements in the contingency table analysis which necessitate the iteration procedure are not present in the analysis of variance.

We may consider the complete sample table to contain all the "information" available from the particular experiment. In the process of analysis, we aim to express the sample table in a reduced number of parameters represented by the marginal totals as expressed in (3.11) to (3.13). In other words, we are interested in knowing how much of this total information is contained in a summary consisting of sets of marginal tables.

If there is no first-order interaction, i.e., independence of all classifications, then all the information is contained in the first-order marginals in the sense that given these marginals, the complete table can be constructed to within sampling error. If the first-order interaction is significant, but there is no second-order interaction, then the set of two-way marginals will be required to summarize the data adequately. The use of two-way tables to summarize multiway classification data is a rather common practice, and the implied assumption is therefore "no second- and higher-order interactions."

A direct consequence of this interpretation is that the analysis can be reduced to that of the set of marginal tables if there is no interaction of the same order.

We remark that the set of marginal tables must be considered jointly for proper interpretation, and if one or more of these tables show significant interactions, the results of tests of the remaining tables could lead to erroneous conclusions. An example of such a case was given in Simpson [1951].

The above interpretation is not restricted to complete sets of marginals. If the p^*-distribution computed from three out of the six two-way marginals in a four-way table is found to be "close enough" to the $\hat{p}$-distribution by our test, the three two-way marginal tables could be considered as containing essentially all the information in the four-way table. The analysis can therefore be performed on these marginal tables and the complexity of the problem reduced. For example, the analysis given in table 3.3 for a four-way table may be reduced to that of one two-way and two three-way tables, and that in table 3.4 to that of three two-way tables and one three-way table, provided that the corresponding interactions are found to be of no significance.

A useful by-product obtained as a result of our computer routine is that the set of residuals, $x-x^*$, are computed for each interaction hypothesis. Inspection and analysis of these residuals may be used as an aid "in assessing the validity or appropriateness of the conventional analysis" as recommended by Anscombe and Tukey [1963], in view of the indefiniteness and complexity of objectives of statistical analysis of multiresponse data.

The analysis of categorical data may well follow this general philosophy and take advantage of some of the developed techniques for the analysis of residuals. In fact, in a goodness-of-fit test, if the computed X^2 shows significance, we usually look at the larger discrepancies between the observed and expected values of the cell frequencies and seek for an explanation. However, this practice has been restricted mainly to one-way tables. A plausible reason for the lack of such study in higher-order tables could be that the computation of expected frequencies becomes complicated

and unmanageable. Consequently, the analysis is considered complete with a formal test of significance.

With the iterative procedure now available for computing the expected frequencies for each particular hypothesis, we could examine these residuals for a number of interesting features, such as:

(a) outliers, or errors in counting and recording,

(b) the physical interpretation of departure from the particular hypothesis,

(c) trend over categories in a classification, particularly if these categories are arranged in a natural sequence of order of magnitude [Cochran 1954, pp. 434–436], and

(d) the agreement of these residuals, squared and weighted by the inverses of the expected frequencies, with the corresponding X^2 distribution.

We have therefore computed and printed these residuals, $x-x^*$, or normalized residuals in table forms as a by product of our computation procedures to facilitate visual examination.

4. Computer Programs and Examples

4.1. Computation and Iteration Programs

The iterative computation process described above for the calculation of cell probabilities, or cell frequencies, representing that of no interaction when certain marginals are considered fixed, is ideally suited for electronic computer operation. A program in Fortran V has been prepared for this purpose.[4] A brief description of this program is given below.

(1) The program is written in double precision mode for the computation of quantities of the form $2\Sigma x \ln x$. These quantities are useful in testing certain hypotheses as illustrated in Kullback, Kupperman, and Ku [1962a, 1962b]. The quantity $0 \ln 0$ is defined as zero.

(2) Input cards are provided for the specification of:

(a) dimension M of the table, and number of categories within each dimension, with $2 \leq M \leq 4$, and $r \times c \times d \times t \leq 10^4$.

(b) maximum number of complete cycles of iterative computation, and the agreement desired between the original given marginals and the computed marginals. Tentatively the maximum number of cycles is set at 20 and the agreement optionally at 0.100, 0.010, and 0.001.

(c) the choice of the set of marginals if these marginals are not a complete set of one-, two-, or three-way marginals. Iterative computation for the complete sets of marginals is automatically performed.

(3) The data cards for the table are read in by column within each row, row × column within each depth, and row × column × depth within each level. Title cards for each of the classifications are provided.

(4) The following notations are used in the output

X(IJKL) original data

Y(IJKL) cell frequencies corresponding to no first-order interaction.

Z(IJKL) cell frequencies corresponding to no second-order interaction.

W(IJKL) cell frequencies corresponding to no third-order interaction.

U1(IJKL), U2(IJKL) } cell frequencies corresponding to specified marginals.

(5) Outputs of the program for a four-way table are in the order listed below. For two- and three-way tables, the input cards will adjust the outputs accordingly.

(a) Titles of classifications.

(b) Original table X(IJKL) in the form of two-way tables.

(c) All marginal three-way, two-way, one-way tables and the grand total.

(d) All 16 sums of quantities of the form $2\Sigma X \ln X$.

---

[4] We are indebted to Mrs. Ruth Varner, Statistical Engineering Laboratory, National Bureau of Standards, for the preparation of this program.

(e) Number of complete cycles of iterations performed and the decimal agreement between marginals.

(f) Tables of normalized residuals $= \{X(IJKL) - Y(IJKL)\}/\sqrt{Y(IJKL)}$

$$2\Sigma_Y \ln_Y$$

$$\text{first-order interaction} = 2\Sigma X \ln X - 2\Sigma Y \ln Y$$

$$\text{chi-squared} = \Sigma \frac{(X-Y)^2}{Y}.$$

(g) Print-outs under (f) are repeated for Z, and W, and for U1, U2 when specified.

Samples of the output are shown in the appendix for the four-way contingency tables used in examples 1 and 2.

4.2. Examples

In the literature there are a number of "classical" examples which have been used to demonstrate tests of no second-order interaction in three-way tables. These examples are collected and listed in table 4.1 where the values of the m.d.i.s. for no second-order interaction are compared with results obtained by other investigators. A number of interesting features are noted.

(1) The maximum number of complete cycles of iteration used was 10 for the $2 \times 2 \times 12$ table due to Snedecor. For the others, 6 to 7 cycles are sufficient for agreement of specified marginals to the third decimal place.

(2) The values of $2\hat{I}$ for no second-order interaction agrees very well with the values of X^2 computed through the solutions of systems of simultaneous equations of third degree, i.e., solutions with 2-way marginals considered as fixed. Solutions based on unrestricted maximum likelihood estimates are, however, somewhat lower than our values.

(3) None of the second-order interactions computed reached the 5-percent level of significance. By the interpretation given in subsection 3.3, conclusions drawn from analysis of the three 2-way marginal tables are valid for the 3-way table.

EXAMPLE 1. Ries and Smith [1963] reported an experiment comparing two detergents, a new product X and a standard product M. The three classifications were water softness, at three levels, temperature, at two levels, and a factor corresponding to previous experience and no previous experience with detergent M. This is a $2 \times 2 \times 2 \times 3$ experiment with

R: preference	$i=1$	X
	2	M
C: water temperature	$j=1$	low
	2	high
D: previous use	$k=1$	nonuser
	2	user
T: water softness	$l=1$	hard
	2	medium
	3	soft

Ries and Smith used a series of chi-squared tests in their paper; Cox and Lauh [1967] reexamined the data recently employing a graphical approach. The data and computations are shown in the print-out sample A in the appendix.

TABLE 4.1. *Comparison of results—second-order interaction in three-way tables*

Example	Value of $2\hat{I}$ with marginal agreement to			Other results		
	0.10	0.01	0.001			
Bartlett [1935] 2×2×2	2.357(4)[a]	2.296(6)	2.294(7)	2.27 2.298 1.93 2.26 2.27 8.89 0.083 7.603	X^2 $2\hat{I}$ X^2 Y^2 Z^2 X^2_m X^2_A $2\hat{I}$	Bartlett. Computed from Bartlett's solution. Goodman [1964b]. Goodman [1964b]. Goodman [1964b]. Koch [1968]. Koch [1968] different model. Kullback [1959, without iteration].
Kastenbaum and Lamphiear [1959] 5×3×2 3×2×5 2×3×5	3.1838(2) 3.1660(4) 3.1609(3)	3.1592(4) 3.1600(5) 3.1591(4)	3.1588(7)	3.158 3.640 3.13 2.8 3.12	X^2 $2\hat{I}$ Y^2 $\hat{Y}^2$ X^2	Kastenbaum [1959] Darroch [1962]. KKK [1962b, without iteration]. Goodman [1964b]. Goodman [1964b]. Plackett [1962].
Snedecor, as quoted on p. 184, Kullback [1959] 2×2×12		7.7157(10)		12.608 15.492 7.59 7.45 7.37 5.18	$2\hat{I}$ $2\hat{I}$ X^2 X^2 Y^2 Z^2	Kullback (without iteration). Kullback (without iteration). Norton [1945]. Goodman [1964b]. Goodman [1964b]. Goodman [1964b].
Kullback [1959], prob. 13.10, p. 188 2×2×2		0.007(5)		0		Theoretical.
Kullback [1959], table 12.2, p. 180 2×4×2		7.584(2)		7.570	$2\hat{I}$	Kullback (algebraic).
Kilkberg, Narragon and Campbell [1964] Bhapkar and Koch 2×2×2			0.0704(5) 0.0430(6) 3.5710(6)	0.071 0.0435 3.3917	X^2_I X^2_e X^2_e	Koch [1968]. Koch [1968]. Koch [1968].
Schotz [1966] Bhapkar and Koch 2×2×4			10.511(7)	7.22	X^2_G	Koch [1968, using index of order association].

[a] Number of complete cycles of iteration.

The analysis of information table corresponding to table 3.1 is shown in table 4.2 below.

TABLE 4.2

Components of information	Information	d.f.
Third-order interaction	0.739	2
$2nI(p_3^*:p_2^*)$	9.108	7
Second-order interaction	9.847	9
$2nI(p_2^*:p_1^*)$	33.081	9
Four-way independence	42.928	18

Neither the third-order nor the second-order interactions reached significance at $\alpha = 0.10$. Hence we conclude that the analysis of the six two-way tables will yield the desired information. The numerical values of these six interactions are computed in two ways for comparison in table 4.3. The first set is computed directly from the six two-way tables. The second set is computed by using the analysis $2nI(p_2^*:p_1^*) = 2\Sigma_{ij} X_{ij..} \ln a_{ij} + \ldots + 2\Sigma_{kl} X_{..kl} \ln f_{kl}$. The sum of the first set, 33.763, should equal the component $2nI(p_2^*:p_1^*)$ in table 4.2. The difference between the two sums represents the effect of the marginal restraints.

TABLE 4.3

Components of information	Information		d.f.
Preference and water temp. $(R \times C)$	4.361	4.393	1
Preference and previous use $(R \times D)$	20.581	19.920	1
Preference and water softness $(R \times T)$	.395	.424	2
Water temp. and previous use $(C \times D)$	1.252	1.314	1
Water temp. and water softness $(C \times T)$	6.099	6.089	2
Previous use and water softness $(D \times T)$	1.075	.943	2
	33.763	33.083	9

The main conclusion here is that preference is highly dependent on previous use, and to a certain extent dependent on the water temperature. The water temperature effect depends somewhat on degree of softness of water. The nonsignificance of $(C \times D)$ and $(D \times T)$ shows that the samples of previous user and nonprevious user of M are not biased with respect to water temperature and water softness.

We also include here analysis of information tables 4.4 and 4.5 corresponding to tables 3.3 and 3.4 respectively.

TABLE 4.4

Components	Information	*d.f.*
$(CT \times R)(D)$	8.059	5
$(CT, R)(D)$	4.185	5
$CT \times R \mid D$	12.244	10

TABLE 4.5

Components	Information	*d.f.*
$(R \times C \times T)(D)$	9.725	7
$(R, C, T)(D)$	10.294	7
$R \times C \times T \mid D$	20.019	14

Since none of these components of information reached significance at $\alpha = 0.10$, we conclude that the interaction between preference and water temperature-water softness are not different for the previous user and nonuser groups. If this conclusion is accepted, then separate analyses of previous user group and nonuser group appear to be unnecessary.

EXAMPLE 2.

For the second sample we use the survey results as reported by Hoyt, Krishnaiah, and Torrance [1959], analyzed also in Kullback, Kupperman and Ku [1962a] for nine hypotheses of independence and conditional independence. The four classifications are:

	Categories
D: high school ranks	3
C: post high school status	4
T: sex	2
R: father's occupational level	7

The data (sample B, appendix) showed considerable heterogeneity and all the nine hypotheses tested in the above analysis gave highly significant results. We continue the analysis in table 4.6. All the interactions are again highly significant excepting the third-order interaction for which $p \doteq 0.15$.

Since the second-order interaction is highly significant, we analyze the difference between second-order and third-order interaction into its component parts in table 4.7, the second set in accordance with the second part of table 3.2. These four components represent second-order interactions in the four three-way tables subject to the three-way marginal restraints. The first set corresponds to the analysis $2nI(p^*:p^*) = 2\Sigma_{ijk}X_{ijk} \cdot \ln a_{ijk} + \ldots + 2\Sigma_{jkl}X_{\cdot jkl} \ln d_{jkl}$.

We note that all the second-order interactions are significant when the R classification is involved, i.e., the interactions $C \times D$, $C \times T$, and $D \times T$ are different for different occupational levels of fathers' occupations. These results, and the fact that there is an unusually larger number of girls than boys for the third level of fathers' occupation as shown in table for $X(I^{**}L)$, suggest that the counts for this level may be suspect.

TABLE 4.6

Components of information	Information	d.f.
$2nI(\hat{p} : p_3^*)$	44.793	36
$2nI(p_3^* : p_2^*)$	127.464	72
$2nI(\hat{p} : p_2^*)$	172.257	108
$2nI(p_2^* : p_1^*)$	3320.858	47
$2nI(\hat{p} : p_1^*)$	3493.115	155

TABLE 4.7

Marginal restraints added	Information		d.f.
All two-way marginals	172.257	172.257	108
RCD	53.841	52.267	36
		119.990	72
RCT	45.161	44.630	18
		75.360	54
RDT	25.477	27.588	12
		47.772	42
CDT	2.985	2.979	6
All three-way marginals	44.793	44.793	36

TABLE 4.8

All two-way marginals		109.521	91
RCD		29.521	30
		80.000	61
RCT		27.738	15
		52.262	46
RDT		11.986	10
		40.276	36
CDT		.673	6
All three-way marginals		39.603	30

Table 4.8 is an analysis of the data with the third level of fathers' occupation deleted. The second-order interaction is still significant at $\alpha = 0.10$, but not at $\alpha = 0.05$. Of the components of second-order interaction, however, only RCT remains significant. The interpretation that the interactions between post high school status and sex are different for different levels of fathers' occupational level appears to be a reasonable one.

We would suggest, therefore, that the data for the third level of fathers' occupation be rechecked.

5. Summary

Using the basic notions of information theory, we have developed in the above sections a unified approach to the analysis of multiway contingency tables. Under this approach the principle of minimum discrimination information is proposed and used to generate hypotheses of interest. It is shown that all classical hypotheses for contingency tables can be generated through the use of this principle when certain marginals are considered fixed.

For each set of fixed marginals, a unique set of cell probabilities $\{p^*\}$ is generated by minimizing the discrimination information. The set of $\{p^*\}$ corresponds to the cell probabilities representing no-interaction, and typically can be expressed in a logarithmic linear form:

$$\ln p^*_{ijk} = \text{const.} + \ln a_{ij} + \ln b_{jk} + \ln c_{ik},$$

where a_{ij}, b_{jk}, and c_{ik} are functions of cell probabilities of the corresponding fixed two-way marginal tables. The difference between the set of cell probabilities estimated from data and $\{p^*\}$ is therefore a measure of interaction.

If the complete set of one-way marginals are considered fixed, the set of $\{p^*_1\}$ represents cell probabilities under the independence hypothesis. If the complete set of two-way marginals are considered fixed, the set of $\{p^*_2\}$ are the cell probabilities representing no second-order interaction. In this sense the higher-order no-interaction hypotheses can be considered as hypotheses of "generalized" independence, a concept which unifies the many attempts in the formulation of second-order interaction described in brief in the introductory section.

The relationship between minimum discrimination information and maximum entropy is examined and the analogy between the proposed analysis and the analysis of variance using least squares theory is noted. An interpretation of the no-interaction hypothesis as equivalent to that "the given marginal tables are sufficient and contain all the information of the full table" reduces the dimension of the table, and hence also the complexity of the analysis.

The expression for p^* for given marginals is given in theorem 2.1 and the convergence of the iterative computation procedure to the unique set of $\{p^*\}$ in theorem 2.2.

Analysis of information tables for four-way tables are given for first-, second-, and third-order interactions, and also for selected mixed-order interactions. A Fortran program to aid in the computation has been prepared.

Two illustrative examples in the analysis of four-way tables are included.

6. Appendix. Samples of Selected Portions of Computer Print-Out

SAMPLE A EXAMPLE 1 (Tables of residuals suppressed)

R	PREFERENCE M OR X	I=1, 2
C	WATER TEMPERATURE	J=1, 2
D	PREVIOUS USER OR NONUSER OF M	K=1, 2
T	WATER SOFTNESS	L=1, 3

312-532 O - 68 - 3

ORIGINAL TABLES

X(IJ11)

68	42
42	30

X(IJ12)

66	33
50	23

X(IJ13)

63	29
53	27

X(IJ21)

37	24
52	43

X(IJ22)

47	23
55	47

X(IJ23)

57	19
49	29

MARGINAL TABLES

THREE-WAY TABLES

X(IJ1*)

197	104	110
145	80	72

X(*J1L)

116	116	105
56	56	66

X(1J*L)

113	120	110
56	48	72

X(I*1L)

99	92	141
73	80	156

X(IJ2*)

66	89	102
119	67	70

X(*J2L)

106	94	105
48	73	70

X(2J*L)

102	61	70
56	95	102

X(I*2L)

76	89	67
78	119	48

TWO-WAY TABLES

X(IJ**)

338	170
301	199

X(I*K*)

301	207
225	275

X(I**L)

171	169	168
167	175	158

X(*JK*)

342	297
184	185

X(*J*L)

199	218	222
139	126	104

X(**KL)

182	172	172
156	172	154

ONE-WAY TABLES

X(I***)

508	500

X(*J**)

639	369

X(**K*)

526	482

X(***L)

338	344	326

TOTAL

X(****)

1008

PRINT OF SUMS

SUM 2X(IJKL)LNX(IJKL)= .7653768886020237 + 004

SUM 2X(IJK*)LNX(IJK*)= .9853563803650491 + 004

SUM 2X(*JKL)LNX(*JKL)= .9018264486617197 + 004

SUM 2X(IJ*L)LNX(IJ*L)= .9017229799353486 + 004

SUM 2X(I*KL)LNX(I*KL)= .8962284823389048 + 004

SUM 2X(IJ**)LNX(IJ**)= .1122496619356278 + 005

SUM 2X(I*K*)LNX(I*K*)= .1116989524449928 + 005

SUM 2X(I**L)LNX(I**L)= .1033087165370435 + 005

SUM 2X(*JK*)LNX(*JK*)= .1122371544867871 + 005

SUM 2X(*J*L)LNX(*J*L)= .1040972402615119 + 005

SUM 2X(**KL)LNX(**KL)= .1033340920997269 + 005

SUM 2X(I***)LNX(I***)= .1254477724916192 + 005

SUM 2X(*J**)LNX(*J**)= .1261792581599639 + 005

SUM 2X(**K*)LNX(**K*)= .1254663500174484 + 005

SUM 2X(***L)LNX(***L)= .1172779757827051 + 005

2N LN N= .1394209847244072 + 005

2Y LN Y= .7610840227851502 + 004
FIRST-ORDER INTERACTION = .4292865816 + 002
CHI-SQUARED = .4390224840 + 002

2Z LN Z= .7643922243020641 + 004
SECOND-ORDER INTERACTION = .9846642999 + 001
CHI-SQUARED= .9870614978 + 001

2W LN W= .7653029670355177 + 004
THIRD-ORDER INTERACTION = .7392156650 + 000
CHI-SQUARED= .7379092751 + 000

SPECIFIED MARGINALS I*K* *JKL
NO. OF ITERATIONS = 1 CYCLE
AGREEMENT BETWEEN MARGINALS TO .100-01

2(U1) LN (U1)= .7641524729371637 + 004
INTERACTIONS (U1)= .1224415664 + 002
CHI-SQUARED= .1220141783 + 002

SPECIFIED MARGINALS I*K* *JKL IJ*L
NO. OF ITERATIONS = 3 CYCLES
AGREEMENT BETWEEN MARGINALS TO .100-01

2(U2) LN (U2)= .7645709639307871 + 004
INTERACTIONS (U2)= .8059246712 + 001
CHI-SQUARED = .8054468429 + 001

SPECIFIED MARGINALS I*K* *JK* **KL
NO. OF ITERATIONS = 1 CYCLE
AGREEMENT BETWEEN MARGINALS TO .100-01

2(U3) LN (U3)= .7633749899660993 + 004
INTERACTIONS (U3)= .2001898635 + 002
CHI-SQUARED = .2069489400 + 002

SPECIFIED MARGINALS I*K* *JK* **KL IJ*L
NO. OF ITERATIONS = 3 CYCLES
AGREEMENT BETWEEN MARGINALS TO .100–01
2(U4) LN (U4)= .7644043799921927 + 004
INTERACTIONS (U4)= .9725086098 + 001
CHI-SQUARED = .9720352364 + 001

SAMPLE B EXAMPLE 2 (Mixed order interactions not shown)

R	FATHER OCCUPATIONAL LEVEL	I = 1, 2, 3, 4, 5, 6, 7
C	POST HIGH SCHOOL STATUS	J = 1, 2, 3, 4
D	HIGH SCHOOL RANKS	K = 1, 2, 3
T	SEX	L = 1, 2

ORIGINAL TABLES

X(IJ11)				X(1J21)				X(IJ31)			
87	3	17	105	216	4	14	118	256	2	10	53
72	6	18	209	159	14	28	227	176	8	22	95
52	17	14	541	119	13	44	578	119	10	33	257
88	9	14	328	158	15	36	304	144	12	20	115
32	1	12	124	43	5	7	119	42	2	7	56
14	2	5	148	24	6	15	131	24	2	4	61
20	3	4	109	41	5	13	88	32	2	4	41

X(IJ12)				X(IJ22)				X(IJ32)			
53	7	13	76	163	30	28	118	309	17	38	89
36	16	11	111	116	41	53	214	225	49	68	210
52	28	49	521	162	64	129	708	243	79	184	448
48	18	29	191	130	47	62	305	237	57	63	219
12	5	10	101	35	11	37	152	72	20	21	95
9	1	15	130	19	13	22	174	42	10	19	105
3	1	6	88	25	9	15	158	36	14	19	93

MARGINAL TABLES

THREE-WAY TABLES

X(1J1*)				X(IJ2*)				X(IJ3*)			
140	10	30	181	379	34	42	236	565	19	48	142
108	22	29	320	275	55	81	441	401	57	90	305
104	45	63	1062	281	77	173	1286	362	89	217	705
136	27	43	519	288	62	98	609	381	69	83	334
44	6	22	225	78	16	44	271	114	22	28	151
23	3	20	278	43	19	37	305	66	12	23	166
23	4	10	197	66	14	28	246	68	16	23	134

THREE-WAY TABLES—Continued

X(*J1L)

365	213
41	76
84	133
1564	1218

X(*J2L)

760	650
62	215
157	346
1565	1829

X(*J3L)

793	1164
38	246
100	412
678	1259

X(1J*L)

559	525
9	54
41	79
276	283

X(2J*L)

407	377
28	106
68	132
531	535

X(3J*L)

290	457
40	171
91	362
1376	1677

X(4J*L)

390	415
36	122
70	154
747	715

X(5J*L)

117	119
8	36
26	68
299	348

X(6J*L)

62	70
10	24
24	56
340	409

X(7J*L)

93	64
10	24
21	40
238	339

X(I*1L)

212	149
305	174
624	650
439	286
169	128
169	155
136	98

X(I*2L)

352	339
428	424
754	1063
513	544
174	235
176	228
147	207

X(I*3L)

321	453
301	552
419	954
291	576
107	208
91	176
79	162

TWO-WAY TABLES

X(IJ**)

1084	63	120	559
784	134	200	1066
747	211	453	3053
805	158	224	1462
236	44	94	647
132	34	80	749
157	34	61	577

X(I*K*)

361	691	774	
479	852	853	
1274	1817	1373	
725	1057	867	
297	409	315	
324	404	267	
234	354	241	

X(I**L)

885	941
1034	1150
1797	2667
1243	1406
450	571
436	559
362	467

X(*JK*)

578	1410	1957
117	277	284
217	503	512
2782	3394	1937

X(*J*L)

1918	2027
141	537
341	891
3807	4306

X(**KL)

2054	1640
2544	3040
1609	3081

ONE-WAY TABLES

X(I***)

1826 2184 4464 2649 1021 995 829

X(*J**)

3945 678 1232 8113

X(**K*)

3694 5584 4690

X(***L)

6207 7761

TOTAL

X(****)

13968

PRINT OF SUMS

SUM 2X(IJKL)LNX(IJKL)= .1419490011041468 + 006

SUM 2X(IJK*)LNX(IJK*)= .1602167221282754 + 006

SUM 2X(*JKL)LNX(*JKL)= .1900742436081673 + 006

SUM 2X(IJ*L)LNX(IJ*L)= .1706458462114764 + 006

SUM 2X(I*KL)LNX(I*KL)= .1680009679212620 + 006

SUM 2X(IJ**)LNX(IJ**)= .1893749331578995 + 006

SUM 2X(I*K*)LNX(I*K*)= .1866950003995916 + 006

SUM 2X(I**L)LNX(I**L)= .1976933167165831 + 006

SUM 2X(*JK*)LNX(*JK*)= .2085192406453136 + 006

SUM 2X(*J*L)LNX(*J*L)= .2189304551608272 + 006

SUM 2X(**KL)LNX(**KL)= .2175298383613909 + 006

SUM 2X(I***)LNX(I***)= .2168255594020366 + 006

SUM 2X(*J**)LNX(*J**)= .2377594145686747 + 006

SUM 2X(**K*)LNX(**K*)= .2363330848251296 + 006

SUM 2X(***L)LNX(***L)= .2474453182056570 + 006

2N LN N= .2666358302324256 + 006

TABLE OF NORMALIZED RESIDUALS

R(IJ11)				R(IJ12)			
−1.162	−.213	2.938	−.481	.155	.113	.552	.616
.671	−.308	1.295	.579	.277	.769	−1.494	−1.404
−1.619	2.262	−2.707	−.476	.664	.178	−.408	1.308
.484	−.156	−.868	.881	.254	−.385	.913	−1.403
1.779	−.916	1.954	−.627	−.734	−.323	−.278	−.060
.116	.062	−.404	−.499	.007	−1.722	1.610	.478
1.519	.996	−.029	.108	−2.067	−1.552	−.246	.216

R(IJ21)				R(IJ22)			
.155	−.947	−.548	−.152	−.434	2.540	−.713	.244
.523	.119	.212	−.251	−.195	.249	.112	−.300
−.835	−.963	−.796	1.344	1.829	−.673	−.580	−.803
−.201	−.207	1.106	.181	−.277	−.329	−.032	−.003
−.139	.523	−1.305	−.402	−1.039	−.831	1.893	.728
−.091	1.735	1.771	−.699	−1.064	.552	−.345	.408
1.925	1.042	1.940	−2.536	−.863	−.754	−.857	1.736

R(IJ31)				R(IJ32)			
1.220	−1.218	−.599	−.225	−.281	−1.242	−.326	.060
−.253	−.737	.162	−1.584	−.527	−.227	−.141	2.448
−.889	−.329	−.084	2.053	.416	.302	2.438	−2.597
−1.224	.555	.004	−.722	1.011	.485	−.801	.675
−.190	−.337	−.198	.842	.373	1.238	−1.661	−.247
.248	.134	−.808	1.027	.659	−.404	−1.182	−.355
.800	.092	−.319	−.359	−1.417	.724	−.063	.653

2Z LN Z = .1417767440958978 + 006 CHI-SQUARED = .1724668778 + 003

SECOND-ORDER INTERACTION = .1722570082 + 003

TABLE OF NORMALIZED RESIDUALS

R(IJ11)				R(IJ12)			
−.384	.383	1.070	−.079	.520	−.216	−.943	.094
−.524	−.937	.835	.290	.818	.763	−.852	−.387
.291	1.084	−.593	−.153	−.280	−.694	.352	.157
.018	−.598	−1.085	.363	−.024	.495	.952	−.463
.620	−.773	1.245	−.509	−.848	.573	−.978	.594
.143	.541	−.863	.097	−.170	−.495	.656	−.103
.513	.491	−.550	−.156	−.953	−.560	.579	.177

R(IJ21)				R(IJ22)			
.023	−.422	−.429	.214	−.026	.174	.332	−.210
−.278	.430	−.736	.417	.334	−.233	.598	−.418
−.150	−.600	.541	.023	.131	.299	−.300	−.021
.103	−.140	.297	−.141	−.113	.081	−.218	.142
.316	1.063	−1.518	.132	−.333	−.523	.947	−.115
.379	−.037	.937	−.421	−.392	.025	−.640	.378
−.038	.252	.879	−.324	.049	−.172	−.665	.249

R(IJ31)				R(IJ32)			
.208	.267	−.623	−.201	−.188	−.082	.363	.158
.628	.484	.210	−1.009	−.532	−.177	−.116	.732
−.037	−.462	−.179	.190	.026	.179	.077	−.142
−.121	.824	.716	−.369	.095	−.328	−.364	.275
−.777	−.452	.750	.608	.655	.171	−.362	−.439
−.451	−.339	−.398	.493	.367	.176	.207	−.358
−.329	−.703	−.656	.786	.329	.356	.370	−.479

2W LN W = .1419042077670569 + 006 CHI-SQUARED = .4418652549 + 002

THIRD-ORDER INTERACTION = .4479333708 + 002

7. References

Anscombe, F. J. and Tukey, J. W. (1963), The examination and analysis of residuals, Technometrics, **5**, 141–160.

Barnard, G. A. (1947), Significance tests for 2×2 tables, Biometrika, **34**, 139–167.

Bartlett, M. S. (1935), Contingency table interactions, J. Roy. Statist. Soc. Supplement **2**, 248–252.

Bhapkar, V. P. (1961), Some tests for categorical data, Ann. Math. Statist. **32**, 72–83.

Bhapkar, V. P. and Koch, G. G. (1965), On the hypothesis of "no interaction" in three-dimensional contingency tables, Institute of Statistics Mimeo Series No. 440, University of North Carolina.

Bhapkar, V. P. and Koch, G. G. (1966), Hypothesis of no interaction in four-dimensional contingency tables, Institute of Statistics Mimeo Series No. 449, University of North Carolina.

Bhapkar, V. P. and Koch, G. G. (1968), Hypothesis of "no interaction" in multidimensional contingency tables, Technometrics, **10**, 107–123.

Birch, M. W. (1963), Maximum likelihood in three-way contingency tables, J. Roy. Statist. Soc. B, **25**, 220–233.

Brown, D. T. (1959), A note on approximations to discrete probability distributions, Information and Control, **2**, 386–392.

Cox, D. R. and Lauh, Elizabeth (1967), A note on the graphical analysis of multidimensional contingency tables, Technometrics **9**, 481–488.

Darroch, J. N. (1962), Interactions in multi-factor contingency tables, J. Roy. Statist. Soc. B, **24**, 251–263.

Deming, W. E. and Stephan, F. F. (1940), On a least squares adjustment of a sampled frequency table when the expected marginal totals are known, Ann. Math. Statist. **11**, 427–444.

Good, I. J. (1963), Maximum entropy for hypothesis formulation, especially for multidimensional contingency tables, Ann. Math. Statist. **34**, 911–934.

Good, I. J. (1965), The Estimation of Probabilities: An Essay on Modern Bayesian Methods, Research Monographs No. 30, The M. I. T. Press, Cambridge, Mass.

Good, I. J. (1966), How to estimate probabilities, J. Inst. Math. Applications **2**, 364–383.

Goodman, L. A. (1964a), Interactions in multidimensional contingency tables, Ann. Math. Statist., **35**, 632–646.

Goodman, L. A. (1964b), Simple method for analyzing three-factor interaction in contingency tables, J. Amer. Statist. Assoc. **59**, 319–352.

Hoyt, C. J., Krishnaiah, P. R., and Torrance, E. P. (1959). Analysis of complex contingency data, J. Exp. Ed. **27**, 187–194.

Ireland, C. T. and Kullback, S. (1968), Contingency tables with given marginals, Biometrika, **55**, 179–188.

Kastenbaum, M. A. and Lamphiear, D. E. (1959), Calculation of chi-square to test the no three-factor interaction hypothesis, Biometrics **15**, 107–115.

Kullback, S. (1959), Information Theory and Statistics (John Wiley &Sons, Inc., New York, N.Y.) (Dover Publications, Inc., New York, N.Y., 1968).

Kullback, S. and Khairat, M. A. (1966), A note on minimum discrimination information, Ann. Math. Statist. **37**, 279–280.

Kullback, S., Kupperman, M., and Ku, H. H. (1962a), Tests for contingency tables and Markov chains, Technometrics **4**, 573–608.

Kullback, S., Kupperman, M., and Ku, H. H. (1962b), An application of information theory to the analysis of contingency tables with a table of 2N ln N, N= 1(1) 10,000, J. Res. NBS **66B** (Math. and Math. Phys.), No. 4, 217–243.

Kupperman, M. (1957), Further applications of information theory to multivariate analysis and statistical inference, Dissertation, Graduate Council of George Washington University.

Lancaster, H. O. (1951), Complex contingency tables treated by the partition of chi-square, J. Roy. Statist. Soc. B **13**, 242–249.

Lewis, B. N. (1962), On the analysis of interaction in multidimensional contingency tables, J. Roy. Statist. Soc. A, **125**, 88–117.

Lewis, P. M. II (1959), Approximating probability distributions to reduce storage requirements, Information and Control, **2**, 214–225.

Lindley, D. V. (1964), The Bayesian analysis of contingency tables, Ann. Math. Statist. **35**, 1622–1643.

Mantel, N. (1966), Models for complex contingency tables and polychotomous dosage response curves, Biometrics **22**, 83–95.

Neyman, J. (1949), Contributions to the theory of the chi-square test, Berkeley Symposium on Mathematical Statistics and Probability, Ed. J. Neyman, Vol. **1**, 239–273, Univ. of Calif. Press, Berkeley.

Norton, H. W. (1945), Calculation of chi-square for complex contingency tables, J. Am. Statist. Assoc. **40**, 251–258.

Plackett, R. L. (1962), A note on interaction in contingency tables, J. Roy. Statist. Soc. B **24**, 162–166.

Rao, C. R. (1965), Linear Statistical Inference and its Applications (John Wiley & Sons, Inc., New York, N.Y.).

Ries, P. N. and Smith, H. (1963), The use of chi-square for preference testing in multidimensional problems, Chemical Engineering Progress **59**, 39–43.

Roy, S. N. and Kastenbaum, M. A. (1956), On the hypothesis of no "interaction" in a multiway contingency table, Ann. Math. Statist. **27**, 749–757.

Simpson, C. H. (1951), The interpretation of interaction in contingency tables, J. Roy. Statist. Soc. B **13**, 238–241.

Wald, A. (1943), Tests of statistical hypotheses concerning several parameters when the number of observations is large, Trans. Am. Math. Soc. **54**, 426–482.

Woolf, B. (1955), On estimating the relation between blood group and disease, Annals of Human Genetics **19**, 251–253.

(Paper 72B3–269)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 3, July–September 1968

On the Coupling of Longitudinal and Transverse Waves in a Linear Three-Element Viscoelastic String Subjected to Transverse Impact

Jack C. Smith and Jeffrey T. Fong [1]

Institute for Materials Research, National Bureau of Standards, Washington, D.C. 20234

(May 10, 1968)

The problem of wave propagation in a simple viscoelastic string subjected to constant velocity transverse impact is reexamined. An error in an earlier solution by Smith (J. Res. NBS **70B**, 257 (1966)) is corrected and an alternate numerical scheme based on the method of characteristics but using an implicit formulation of finite-difference equations is presented. The constitutive equation used is that of a linear viscoelastic model consisting of a spring and Maxwell element in parallel. Results of an illustrative calculation are discussed.

Key Words: Characteristics; finite-difference equations; linear viscoelasticity; partial differential equations; transverse impact; wave propagation; waves in strings.

1. Introduction

The theoretical problem of wave propagation in a uniform string subjected to oblique impact is well understood if one assumes a dynamic stress-strain relation $T=T(\epsilon)$ for the material, where T denotes the tensile force acting along the string, ϵ, the Lagrangian strain, and there is no explicit dependence of T on the rate of strain.

Several types of mathematical complication can enter into this theory. The first type is due to the nonlinearity of the function $T(\epsilon)$. The theory predicts that:

(a) if the curve $T(\epsilon)$ is concave towards the ϵ axis, strains of increasing magnitude are propagated with decreasing velocity c given by

$$c=\sqrt{\frac{1}{m}\frac{dT}{d\epsilon}} \tag{1}$$

where m denotes the mass of the string per unit of unstrained length, and

(b) if the curve $T(\epsilon)$ contains a portion that is concave towards the T axis the strain distribution is discontinuous, containing a strong shock, or group of strains propagating at the same velocity.

Another type of complication arises when the string is allowed to undergo arbitrary spacial motion. Even though the theory is restricted to one-dimensional strain, the velocity at every point of the string is a three-dimensional vector which can be resolved into tangential and normal components representing longitudinal and transverse motions respectively. Depending on the initial shape of the string and the boundary conditions, the two wave motions may be coupled in

[1] N.R.C.–N.B.S. Postdoctoral Resident Research Associate, 1966–68.

the sense that no simple wave solution for each motion can be found. Two characteristic velocities are involved: different values of strain in the longitudinal wave are propagated at velocity c given by (1), and changes in configuration of the string are propagated at different values of the velocity P given by

$$P=\sqrt{\frac{1}{m}\frac{T}{1+\epsilon}} \tag{2}$$

For a detailed discussion of this rate-independent theory as applied to string motion, see Cristescu [1, 2].[2]

The complication in the coupling of the two motions is avoided when one considers an infinitely long string, initially straight and subjected to a constant-velocity transverse impact. Simple wave solutions were reported by Smith, McCrackin, and Schiefer [3], and were recently given in another form by Schultz, Tuschak, and Vicario [4]. Attempts to interpret the results of transverse impact experiments on materials such as nylon and polyester yarns, and strips of natural rubber, based on the rate-independent theory, however, were not completely satisfactory. In particular, two basic predictions of the theory were not verified:

(a) The quasistatic and dynamic stress-strain curves of the nylon and polyester samples tested by Petterson and Stewart [5, 6] and by Smith, Fenstermaker, and Shouse [7], have portions concave towards the tension axis, implying that strong shocks should exist in the strain distributions. Neither group noted the presence of any strong discontinuities in their experimental data.

(b) For each impact velocity, the theory yields a unique relation between the strain and the longitudinal wave velocity $c(\epsilon)$. It is an inherent feature of the rate-independent theory that this unique relation is valid for all impact velocities. Experimental data failed to support this assertion after appropriate consideration was given to measurement uncertainties. For additional discussion, see Smith and Fenstermaker [8].

In order to gain insight for interpreting these effects it is useful to study the behavior under impact conditions of a simple linear viscoelastic model, such as one consisting of a spring in parallel with a Maxwell element.[3] This model has already been used by Morrison [9] and Smith [10] to study wave propagation in filaments impacted longitudinally. By analogy with results obtained in these theoretical studies, the effects of viscoelasticity on experimentally obtained strain, tension, and particle velocity distributions are better understood. By extending the use of this model to the transverse–impact problem, further enlightenment will result. In a viscoelastic string it is not possible to uncouple the mutual influence of the two types of wave as was done in the rate-independent theory under some restrictive assumptions. Thus one must study theoretically such additional effects of viscoelasticity as changes in the transverse wave profile, changes in the transverse wave propagation velocity, and secondary changes in the strain, tension, and particle velocity distributions.

A detailed analysis of such a problem with a proposed numerical scheme suitable for the calculation of strong discontinuities was published by Smith [11]. Since publication several errors have been found with the consequence that the proposed numerical scheme is not valid, although the basic formulation of the problem and the mathematical method of solution remain applicable. In this paper these errors are corrected and the numerical scheme revised. In addition the problem is discussed from a different viewpoint and an alternate numerical scheme presented. Illustrative numerical calculations are also given.

---

[2] Figures in brackets indicate the literature references at the end of this paper.

[3] It should be noted that for three-dimensional problems there are objections to the use of constitutive equations characterizing the behavior of spring and dashpot models. Unless properly formulated, such equations, containing time derivatives of the stress and strain, violate the so-called "principle of material indifference" as stated by Truesdell and Toupin [12]. However, the restrictions imposed by this principle are automatically satisfied in the one-dimensional problem considered here.

2. Notation

The symbols used are the same as those used in reference [11] except for the symbol K representing the spring constant.

m initial density of the string in mass per unit length.

K spring constant of the string in force units.

λ dimensionless parameter having a value between 0 and 1 such that λK is the spring constant of the Maxwell element constituting one branch of the viscoelastic model.

τ relaxation time of the Maxwell element.

c velocity of the longitudinal wavefront as given by eq (1); for the three-element model it is given by $c=\sqrt{K/m}$.

T tension in the string in force units.

P velocity related to the propagation of transverse waves as given by eq (2).

V transverse impact velocity.

t time coordinate.

x Lagrangian space coordinate fixed to the string.

x', y' laboratory or observer's coordinates to be referred to as horizontal and vertical coordinates, respectively; the x and x' coordinates of the string coincide in the initial unstrained state.

ξ, η horizontal and vertical components of displacement of a point x on the string relative to its original position:

$$x'=x+\xi(x,t);\ y'=\eta(x,t). \tag{3}$$

u, v horizontal and vertical components of velocity in x', y' space of a point x on the string:

$$u=\frac{\partial x'}{\partial t}=\frac{\partial \xi}{\partial t};\ v=\frac{\partial y'}{\partial t}=\frac{\partial \eta}{\partial t}. \tag{4}$$

α, β first partial derivatives of the laboratory coordinates of a point x on the string with respect to the Lagrangian coordinate x:

$$\alpha=\frac{\partial x'}{\partial x}=1+\frac{\partial \xi}{\partial x};\ \beta=\frac{\partial y'}{\partial x}=\frac{\partial \eta}{\partial x}. \tag{5}$$

ds infinitesimal length element of the deformed string:

$$ds=\sqrt{(dx')^2+(dy')^2}=\sqrt{\alpha^2+\beta^2}\,dx. \tag{6}$$

ϵ Lagrangian strain at x on the string

$$\epsilon=\frac{ds-dx}{dx}=\sqrt{\alpha^2+\beta^2}-1. \tag{7}$$

θ angle that each infinitesimal length element makes with the horizontal x' direction:

$$\cos\theta=\frac{\partial x'}{\partial x}\frac{dx}{ds}=\frac{\alpha}{1+\epsilon};\ \sin\theta=\frac{\beta}{1+\epsilon}. \tag{8}$$

w flow or particle velocity of a point x on the string with respect to an inextensible coordinate coinciding with the string and fixed to it at points in advance of the longitudinal-wave front; that is, the rate of extension of the portion of string between point x and the longitudinal-wave front. This velocity satisfies the differential equation:

$$dw = du\cos\theta + dv\sin\theta = \frac{\alpha}{1+\epsilon}du + \frac{\beta}{1+\epsilon}dv. \tag{9}$$

3. Formulation

The viscoelastic model consists of a spring of spring constant $(1-\lambda)K$ in parallel with a Maxwell element of spring constant λK and relaxation time τ. If the quantity mc^2 is substituted for K, the constitutive equation for this model takes the form

$$mc^2\frac{\partial\epsilon}{\partial t} + \frac{(1-\lambda)mc^2}{\tau}\epsilon = \frac{\partial T}{\partial t} + \frac{1}{\tau}T. \tag{10}$$

For plane motion the following two equilibrium equations apply:

$$m\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(T\cos\theta) = \frac{\partial}{\partial x}\left[\frac{\alpha T}{1+\epsilon}\right] \tag{11}$$

$$m\frac{\partial v}{\partial t} = \frac{\partial}{\partial x}(T\sin\theta) = \frac{\partial}{\partial x}\left[\frac{\beta T}{1+\epsilon}\right]. \tag{12}$$

The equations of continuity are

$$\frac{\partial u}{\partial x} = \frac{\partial\alpha}{\partial t} \tag{13}$$

$$\frac{\partial v}{\partial x} = \frac{\partial\beta}{\partial t}. \tag{14}$$

We shall consider only the waves propagating in the positive x direction. The solution therefore of the set of eqs (7), (9), and (10) through (14) must satisfy the initial conditions: for $t=0$, $x>0$

$$u=v=w=\beta=\epsilon=T=0,\ \alpha=1, \tag{15}$$

and the boundary conditions: for $t>0$, $x=0$

$$u=0,\ v=V, \tag{16}$$

and for $t>0$, $x\to\infty$

$$u=v=w=\beta=\epsilon=T=0,\ \alpha=1. \tag{17}$$

In addition to the initial and boundary conditions, certain compatibility conditions also apply. At the longitudinal wave front ϵ, w, and T are discontinuous and must satisfy the jump relations

$$[w] = -c[\epsilon] \tag{18}$$

$$[T] = -mc[w] \tag{19}$$

where the bracketed quantities represent jumps in value occasioned by the passage of the wave front at the point under consideration. At the transverse wave front u, v, α, β, are discontinuous and must satisfy the jump relations

$$[u] = -P[\alpha-1] \tag{20}$$

$$[v] = -P[\beta]. \tag{21}$$

4. Explicit Method of Solution

The variables u, v, α, β can be eliminated from eqs (7), (9), and (11) through (14) to obtain the equations

$$\frac{\partial w}{\partial t}=\frac{1}{m}\frac{\partial T}{\partial x} \tag{22}$$

$$\frac{\partial w}{\partial x}=\frac{\partial \epsilon}{\partial t}. \tag{23}$$

These equations and the constitutive eq (10) form a set having characteristics given by

$$\frac{dx}{dt}=\pm c \tag{24}$$

and

$$\frac{dx}{dt}=0. \tag{25}$$

Thus, the strain ϵ, tension T, and particle velocity w can have discontinuities only along the characteristic curves $x=\pm ct+a$, and $x=b$, in which a and b are constants of integration. In particular, ϵ, T, and w are discontinuous at the longitudinal wave front, but are continuous at the transverse wave front.

The following equations hold along the characteristics: For the "$+c$" characteristic

$$mcdw-dT=[T-(1-\lambda)mc^2\epsilon]\frac{dt}{\tau}; \tag{26}$$

for the "$-c$" characteristic

$$mcdw+dT=-[T-(1-\lambda)mc^2\epsilon]\frac{dt}{\tau}; \tag{27}$$

for the "$x=b$" characteristic

$$mc^2d\epsilon-dT=[T-(1-\lambda)mc^2\epsilon]\frac{dt}{\tau}. \tag{28}$$

Equation (28) is the same as the constitutive eq (10).

The values of the strain, tension, and particle velocity at the longitudinal wave front can be found by solving the set of equations (18), (19), and (26). The results are

$$\epsilon(ct,\ t)=\epsilon_0 e^{-(\lambda t/2\tau)} \tag{29}$$

$$T(ct,\ t)=mc^2\epsilon_0 e^{-(\lambda t/2\tau)} \tag{30}$$

$$w(ct,\ t)=-c\epsilon_0 e^{-(\lambda t/2\tau)}, \tag{31}$$

where ϵ_0 is the strain $\epsilon(0,\ 0)$ resulting at the instant of impact. To find the value of ϵ_0, the compatibility conditions (20) and (21) are expressed in the form

$$u=w+P(1+\epsilon-\alpha) \tag{32}$$

$$v=-P\beta \tag{33}$$

in which the values of u, v, α, and β are understood to be the values obtained just after passage of the transverse wave front, and the continuous quantities P, ϵ, and w are also evaluated at the wave front. Applying the boundary conditions (16) to eqs (18), (32), and (33), and using eq (7), one finds that at the point of impact the relation $V^2=P_0^2(1+\epsilon_0)^2-[(1+\epsilon_0)P_0-c\epsilon_0]^2$ must be satisfied. From eqs (2), (18), and (19), one obtains $P_0=c\sqrt{\epsilon_0/(1+\epsilon_0)}$ which, when substituted into the relation above, gives

$$V^2/c^2=\epsilon_0(1+\epsilon_0)-[\sqrt{\epsilon_0(1+\epsilon_0)}-\epsilon_0]^2. \tag{34}$$

The value of ϵ_0 is obtained by solving eq (34).

If velocity P is defined as in eq (2), it is obvious that eqs (11) through (14) form a set involving P and the dependent variables u, v, α, and β. This set of equations has characteristics given by

$$\frac{dx}{dt}=\pm P \tag{35}$$

and along these characteristics the following relations hold: For the "$+P$" characteristic,

$$\beta(du-Pd\alpha)-\alpha(dv-Pd\beta)=0, \tag{36}$$

and for the "$-P$" characteristic,

$$\beta(du+Pd\alpha)-\alpha(dv+Pd\beta)=0. \tag{37}$$

The solution of the system of equations (7), (9), (26), (27), (28), (36), and (37), is found by numerical integration along the set of characteristics plotted in the Lagrange diagram, figure 1. In this diagram the straight line characteristics are solutions of the equation $dx/dt=\pm c$; the characteristic passing through the origin, and having the equation $x=ct$ corresponds to the discontinuity marking the wave front of the strain, tension, and particle velocity distributions. Thus, in region 0 between this characteristic and the x axis the strain ϵ, tension T, and particle velocity w are zero. Along the region 1 side of the characteristic the values of ϵ, T, and w are given by eqs (29), (30), and (31), which may be thought of as boundary conditions.

The curved line passing through the origin represents a solution of the equation $dx/dt=P$. The exact course of this characteristic is not known in advance, as P is a function of ϵ and T. This characteristic corresponds to the front of the wave of transverse motion that propagates along the filament; thus, in region 1 between this characteristic and the characteristic $x=ct$ the velocity u is equivalent to the velocity w, the variable α is equal to $1+\epsilon$, and the velocity v and variable β are equal to zero. The jump relations (32) and (33) holding along the transverse wave front constitute a second set of boundary conditions. A third set of boundary conditions expressed by eq (16) holds along the time axis.

Calculation of values for u, v, w, α, β, ϵ, T at the mesh points in the Lagrangian diagram (using fig. 1 as an example) proceeds systematically in the following steps:

1. Calculate ϵ_0 using eq (34).
2. Calculate w, ϵ, T for mesh points along the characteristic $x=ct$, using eqs (29), (30), and (31).
3. Calculate w, α, β, ϵ, T at point 1, and u, v, w, α, β, ϵ, T at point 2 using a subroutine to be described later.
4. Calculate u, v, w, α, β, ϵ, T at successive points 3, 4, 5, 6.
5. Calculate w, ϵ, T at successive points a, b, c, etc.
6. Continue the calculation as indicated.

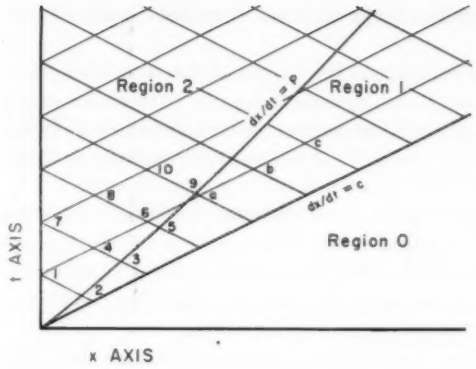

FIGURE 1. *Characteristics network used in the explicit method of solution.*

The straight line characteristics of positive and negative slope are solutions of the eq $dx/dt = \pm c$. The characteristic separating region 1 from region 0 gives the location of the longitudinal wave front. The curve characteristic separating region 2 from region 1 and satisfying the eq $dx/dt = P$ gives the location of the transverse wave front.

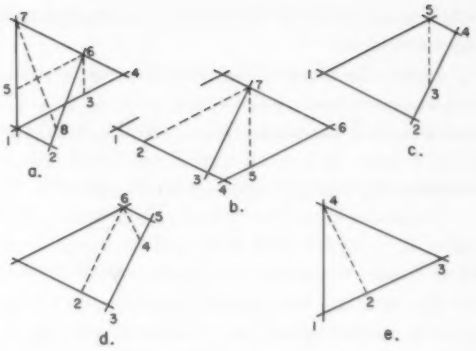

FIGURE 2. *Mesh situations encountered during integration along the characteristics plotted in figure 1.*

Five mesh situations depicted in figure 2 are encountered in the numerical integration process. The simplest of these is that of figure 2c. Here, points 1 and 5 lie at the intersections of c characteristics, and the characteristic between points 2 and 4 may be either a c or a P characteristic; line (3, 5) is a constructed vertical line. Values of w, ϵ, and T at point 5 are found from data known at points 1, 2, and 4 by solving eqs (26), (27), and (28) written respectively in the form

$$mcw - T = mcw_1 - T_1 + [T_{15} - (1-\lambda)mc^2E_{15}](t_5 - t_1)/\tau \tag{38}$$

$$mcw + T = mcw_4 + T_4 - [T_{45} - (1-\lambda)mc^2E_{45}](t_5 - t_4)/\tau \tag{39}$$

$$mc^2\epsilon - T = mc^2\epsilon_3 - T_3 + [T_{35} - (1-\lambda)mc^2E_{35}](t_5 - t_3)/\tau. \tag{40}$$

In these equations the symbol T_{15}, for example, represents the average value of $(T_1 + T)/2$. In the first trial calculation T_{15} is set equal to T_1; the calculation is repeated twice using improved values of T_{15}.

Figure 2a depicts a situation found in meshes low on the t axis. In the lowest mesh the transverse wave front characteristic passes through the origin so that points 1 and 2 coincide, but at later times the more general form depicted may occur. Values of u, v, w, α, β, ϵ, T, x, and t at point 6 and w, α, β, ϵ, and T at point 7 are required. The large set of equations involved is most conveniently solved by an iterative process in which it is assumed initially that the value of w at point 7 is equal to the value of w at point 1. This enables ϵ, and T at point 7 to be calculated using eq (28) along the time axis (1, 7) and eq (27) along characteristic (4, 7) (segment (6, 7) in subsequent iterations).

The transverse wave front characteristic is constructed with slope $1/P$ evaluated from point 2 data. The vertical line (3, 6) and the characteristic (5, 6) are then constructed and values of w, ϵ, and T at points 3 and 5 determined by interpolation. Values of w, ϵ, and T are calculated at point 6 using eq (26) along (5, 6), eq (27) along (4, 6), and eq (28) along (3, 6). Values of u, v, α, and β are found using eq (36) along the transverse wave front characteristic (2, 6) and the compatibility relations (32) and (33) plus eq (7) applied at point 6. Characteristic (7, 8) is then constructed with slope $(-1/P)$ evaluated from point 7 data. The values of α and β at point 7 are found by applying eq (37) along (7, 8) and eq (7) at point 7. The iteration cycle is completed by finding w at point 7 through use of eq (9) along line segment (6, 7). Improved values of the required quantities are obtained by iterations which are continued until successive values of w at point 7 are found to differ by a suffi-

312-532 O - 68 - 4

ciently small amount. During the calculation subiterations of the type discussed for situation 2*c* are also carried out.

Figure 2b depicts the situation encountered in tracing out the course of the transverse wave front characteristic; values of u, v, w, α, β, ϵ, T, x, and t are required at point 7. In this case values of w, ϵ, and T are found from relations holding along (6, 7) and the two constructed lines (2, 7) and (5, 7). Values of u, v, α, and β are found using eq (36) along (3, 7) and applying the compatibility relations (32) and (33) plus eq (7) at point 7.

Situation 2*d* occurs when values of u, v, α, and β at point 6 are calculated from data known at points 1, 3, and 5, and from values of w, ϵ, and T at point 6. The characteristic between points 3 and 5 may be either a c characteristic or the transverse wave front characteristic. In this case, eqs (36) and (37) are applied respectively along the constructed P characteristics (2, 6) and (4, 6), eq (9) is applied along the c characteristic (5, 6), and eq (7) is applied at point 6.

In situation 2*e* values of w, α, β, ϵ, and T at point 4 on the time axis are calculated from data at points 1 and 3 on a c characteristic. In the solution of this problem, eq (28) is applied along the time axis, eq (37) along the constructed P characteristic (2, 4), eqs (9) and (27) along the c characteristic (3, 4), and eq (7) at point 4.

In order to find the configuration of the filament in laboratory (x', y') coordinates, it is desirable to know the values of ξ and η at each of the mesh points in the Lagrange diagram. Along the longitudinal wave front the values of ξ and η are zero, and along the transverse wave front the value of η is zero. The value of ξ is continuous across the transverse wave front. In region 1 the value of η is zero and the value of ξ is found in terms of w and ϵ by integrating along a negative c characteristic using the relation

$$\frac{d\xi}{dt}=\frac{\partial\xi}{\partial t}+\frac{dx}{dt}\frac{\partial\xi}{\partial x}$$

which becomes, after appropriate substitutions

$$d\xi=(w-c\epsilon)dt. \tag{42}$$

In region 2, ξ and η are found by integrating along a negative c characteristic using the relations

$$d\xi=[u-c(\alpha-1)]dt \tag{43}$$

$$d\eta=(u-c\beta)dt. \tag{44}$$

5. Errors in a Previous Solution

The scheme just presented has been outlined in more than the usual detail because it avoids several errors occurring in a previous solution [11]. Most of these errors were due to improper use of eq (9). It should be noted that eq (9), upon substitution of the boundary values for u and v at $x=0$, reduces to the relation $(\partial w/\partial t)_{x=0}=0$. This implies erroneously that w is constant along the time axis. The mistake occurs because in this application of eq (9) w has been expressed relative to a coordinate system fixed to the string at the point of impact, but the value of w desired is that relative to a system fixed to the string at points in advance of the strain wave front. A similar error results if eq (9) is applied along the transverse wave front characteristic.

Another erroneous result is obtained if, in situation 2*e*, eq (9) is applied along the negative P characteristic to find the value of w at point 4. In this example the value of w at point 2 is obtained by interpolation between values at points 1 and 3. Thus, the relation (9) is split into two components one of which is applied along the t axis. situation 2*a* provides a similar opportunity to make this mistake.

Equation (7) can be expressed in the differential form

$$\alpha d\alpha + \beta d\beta = (1+\epsilon)d\epsilon \tag{45}$$

which is more convenient for calculation. Its use in this form, however, is unnecessary, and produces a small cumulative error.

If eqs (36) and (37) are combined with eqs (9) and (45), the following relations are obtained along the "$+P$" characteristics:

$$du - Pd\alpha = \frac{\alpha}{1+\epsilon}(dw - Pd\epsilon) \tag{46}$$

$$dv - Pd\beta = \frac{\beta}{1+\epsilon}(dw - Pd\epsilon); \tag{47}$$

and along the "$-P$" characteristics:

$$du + Pd\alpha = \frac{\alpha}{1+\epsilon}(dw + Pd\epsilon) \tag{48}$$

$$dv + Pd\beta = \frac{\beta}{1+\epsilon}(dw + Pd\epsilon). \tag{49}$$

However, these relations, used previously [11], have yielded inaccurate and often erroneous results. They are, for instance, invalid along the transverse wave front characteristic when used in connection with eq (7) or (45), and invalid along the "$-P$" characteristic in situations 2*a* and 2*e*. In situation 2*d* eqs (46) through (49) have yielded inaccurate results, especially in those meshes involving the transverse wave front characteristic.

6. Coupling Between Longitudinal and Transverse Waves

It is interesting to note that of the two wave phenomena present, the longitudinal wave is described in terms of the quantities ϵ, w, and T, and the transverse wave in terms of the quantities u, v, α, and β. It has been shown that the differential equations describing the problem can be reduced to a set involving w, ϵ, and T only; thus, it would seem that values of w, ϵ, and T could be found separately, and in a second step values of u, v, α, and β found in terms of them. Unfortunately, however, the boundary conditions are expressed in terms of the variables u and v so that in general this decoupling is impossible.[4]

From a physical point of view the effects of coupling between the variables describing the the longitudinal and transverse waves can be described as follows: Changes in the strain, tension, and particle velocity distributions due to viscoelasticity induce changes in the configuration and propagation velocity of the transverse wave which react back to modify the strain, tension, and particle velocity distributions. Thus, the viscoelastic effects can be considered as both primary and secondary.

The distributions resulting from the primary effect, are the same as those resulting from a longitudinal impact at constant velocity, in which the strain increases, the tension decreases, and the particle velocity stays constant at the point of impact. In the secondary or coupling effect the particle velocity at the point of impact changes with time, and associated changes occur in the strain, tension, and particle velocity distributions. If viscoelasticity is absent, as when the constitutive equation is of form $T = T(\epsilon)$, and if transverse impact occurs at constant velocity, only the primary effect is involved, and no changes occur in the longitudinal and transverse waves. In this case the problem may be considered as effectively decoupled.

[4] In the previous paper [11] eq (9) was applied along the t axis and the erroneous result $w = a$ *constant* used as a boundary condition to achieve decoupling.

7. Implicit Method of Solution

In the method of solution discussed above, explicit systems of equations are used to evaluate the unknowns at successive points in a characteristics network. Alternatively, values of the unknowns at points along the string can be calculated simultaneously by the following algorithm, based on an implicit finite-difference formulation for nonlinear wave propagation problems [13].

In order to simplify the calculation, the mathematical problem is reformulated in terms of the five unknowns u, v, α, β, and T. The two additional unknowns, ϵ and w, are defined by eqs (7) and (9), and can be found separately. The equations are the same as those used in the first method; namely, eqs (26) and (27) holding along the $\pm c$ characteristics, the constitutive eq (28), and eqs (36) and (37) holding along the $\pm P$ characteristics, except that the variables ϵ and w have been evaluated in terms of the variables u, v, α, and β, and do not appear.

The mesh system used is depicted in figure 3. As before, there are three regions of interest: region 0 for points in advance of the longitudinal wave front, region 1 for the portion of the longitudinal wave in advance of the transverse wave front, and region 2 for points within the transverse wave. The differential equations have different forms in regions 1 and 2. In region 1 there are no P characteristics and the variables v and β are both equal to zero; thus only eqs (26), (27), and (28) with $\alpha-1$ substituted for ϵ and u substituted for w are used here. The more general forms of the equations with $\sqrt{\alpha^2+\beta^2}-1$ substituted for ϵ and $(\alpha du+\beta dv)/\sqrt{\alpha^2+\beta^2}$ substituted for dw are used in region 2. Along the longitudinal wave front the values of u, α, and T are found from eqs (29), (30), and (31) by substituting $\alpha-1$ for ϵ and u for w, and along the t axis the values of u and v are given by the boundary condition (16). Along the transverse wave front characteristic four compatibility conditions are needed. These are:

$$u_2=u_1-P(\alpha_2-\alpha_1) \tag{50}$$

$$v_2=-P\beta_2 \tag{51}$$

$$T_2=T_1 \tag{52}$$

$$\alpha_2^2+\beta_2^2=\alpha_1^2 \tag{53}$$

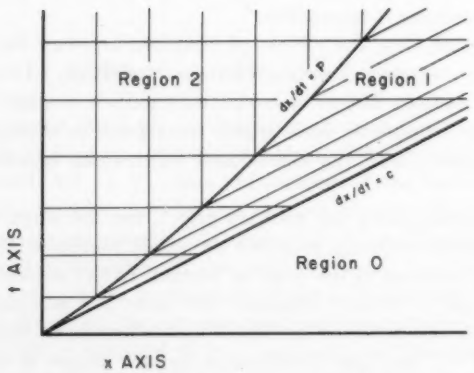

FIGURE 3. *Mesh system used in the implicit method of solution.*

The Δx increments of the mesh are constant in region 2. The Δx increments in region 1 and Δt increments in regions 1 and 2 are variable, depending on the value of the velocity P at the transverse wave front.

where the subscripts refer to values of the variables in the regions 1 and 2. Equations (50) and (51) are the same as the compatibility conditions (20) and (21), and eqs (52) and (53) merely state mathematically that the tension and strain are continuous across the transverse wave front as was shown earlier in the text. Alternatively, eqs (52) and (53) may be obtained by equating horizontal and vertical components of the force across the transverse wavefront [3] or by the matrix methods expounded by Jeffrey and Taniuti [14].

In the mesh system the distance increment Δx is maintained constant in region 2, and a variable time increment is defined as $\Delta t = \Delta x/P$ where P is the transverse wave front velocity averaged between points (x, t) and $(x+\Delta x, t+\Delta t)$. In region 1 the distance increment depends on the value of P and thus is variable also. The value of P as a function of x and t is not known in advance, so the mesh system can only be constructed in stages as the calculation proceeds.

The calculation is carried out in a series of timewise steps in which the values of u, v, α, β, and T at each mesh point corresponding to $t+\Delta t$, are found in terms of values of these quantities known at each mesh point corresponding to time t. In the calculation each of the timewise steps is iterated several times in order that the trajectory of the transverse wave front (and value of P) be known with sufficient accuracy.

Two types of calculation, represented schematically in figure 4, occur in each step. The simplest of these, figure 4a, is used in region 1 to calculate values of u, α, and T at point 6 in terms of values known at points 1, 2, and 5. In this calculation vertical line (3, 6) and line (4, 6) of slope $(-1/c)$ are constructed, and the values of u, α, and T at points 3 and 4 determined by interpolation. The required values at point 6 are found by solving the equations holding along the characteristics (1, 6), (3, 6), and (4, 6). The calculation is applied sequentially starting at the longitudinal wave front characteristic and working towards the transverse wave front characteristic.

The subcalculation, figure 4b, is used to find values of u_1, u_2, v_1, v_2, α_1, α_2, and T at point a on the transverse wave front and values of u, α, and T at the mesh points in region 2 corresponding to time $t+\Delta t$. The subscripts refer to regions 1 and 2 separated by the transverse wave front characteristic. For the seven unknown quantities at point a there are seven corresponding equations, four holding along the characteristics (b, a), (c, a), (d, a), and (e, a) plus the three compatibility conditions (50), (51), and (53). Values of u, v, α, β, and T are not known at point e however, so the values required at point a cannot be determined explicitly by solving these seven equations. To find the five values required at point e it is necessary to know the corresponding values at point f, and this requires the introduction of five equations holding along the c characteristics (g, f) and (j, f), the P characteristics (h, f) and (i, f), and the line (d, f). Similarly, additional equations are required for each of the mesh points in region 2. The final point p lies on the t axis and is evaluated from three equations holding along (q, p), (r, p), and (s, p) plus the boundary conditions $u=0$, and $v=V$. In this way a large system of simultaneous equations is obtained, the solution of which gives the required values at each of the mesh points.

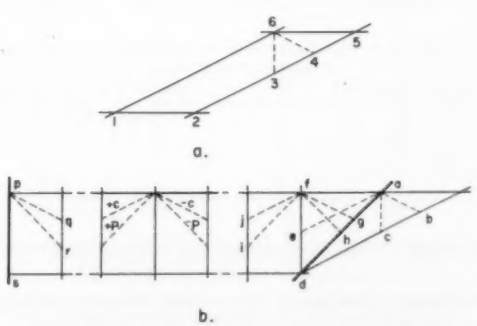

FIGURE 4. *Mesh situations encountered in the implicit method of solution*

This alternate formulation has several advantages. A fundamental set of equations is used in which the number of unknowns is equal to the number of relations holding along the characteristics. This set of five equations in u, v, α, β, and T is well posed for the prescribed initial and boundary conditions. Moreover, implicit schemes of this type are known to be stable at large values of time. Ordinarily, implicit schemes do not require small time steps in regions where the characteristics are nonlinear, but in this application the presence of a moving boundary of unknown curvature (transverse wave front characteristic) may limit this latter advantage.

8. Calculated Results

The explicit method has been used to calculate the behavior of the viscoelastic string for various values of the parameters λ, m, c, and τ characterizing the model and for various values of the transverse impact velocity V. The results for one of these calculations with parameters $\lambda = 0.2$, $m = 100\ \text{gm}^{-1}$, $\tau = 0.002$ s, $c = 100\ \text{ms}^{-1}$, and $V = 50\ \text{ms}^{-1}$ are presented here. The values chosen for the parameters roughly simulate the material properties of an elastomer such as rubber when subjected to transverse impact.

The distributions of the particle velocity, strain, and tension calculated in this example are shown in figures 5, 6, and 7, respectively. The ordinate in figure 5 is a dimensionless quantity, the ratio of the particle velocity at a Lagrangian distance x along the string to the particle velocity at the instant of impact, w/w_0. The distribution of particle velocity in the wave is shown by the solid line curves for times of 1, 2, 3, 4, and 5 ms after impact. The dashed lines indicate the velocity distribution for the case of no relaxation ($\lambda = 0$). The distributions are similar to those resulting from longitudinal impact at constant velocity [10] except that in this example the particle velocity at the origin increases with time slightly, whereas in the case of longitudinal impact it necessarily remains constant. This illustrates the effect of coupling between the longitudinal and transverse waves when viscoelasticity is present.

The dimensionless ordinate in figure 6 is the ratio of the strain at a distance x to the strain at the instant of impact, ϵ/ϵ_0. The distributions depicted are similar to those resulting from longitudinal impact at constant velocity. The strain at the point of impact increases with time and approaches a limiting value, but this limiting value is greater than the value of $\epsilon_0(1-\lambda)^{-1/2} = 1.118\epsilon_0$ which is

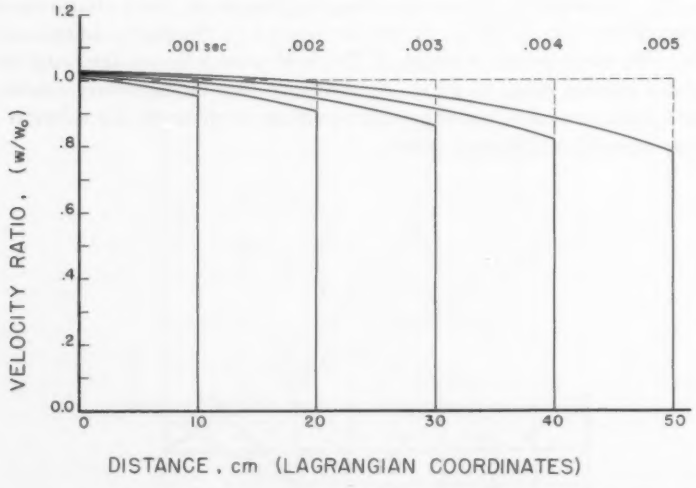

FIGURE 5. *Distribution of particle or flow-velocity along the string for times of 1, 2, 3, 4, and 5×10^{-3} s after transverse impact.*

Calculation parameters are $\lambda = 0.2$, $m = 100\ \text{gm}^{-1}$, $c = 100\ \text{ms}^{-1}$, $\tau = 0.002$ s, and $V = 50\ \text{ms}^{-1}$. Dash lines give distributions for an elastic string ($\lambda = 0$). The particle velocity is expressed as the ratio of the velocity w at distance x to the velocity w_0 attained at the instant of impact.

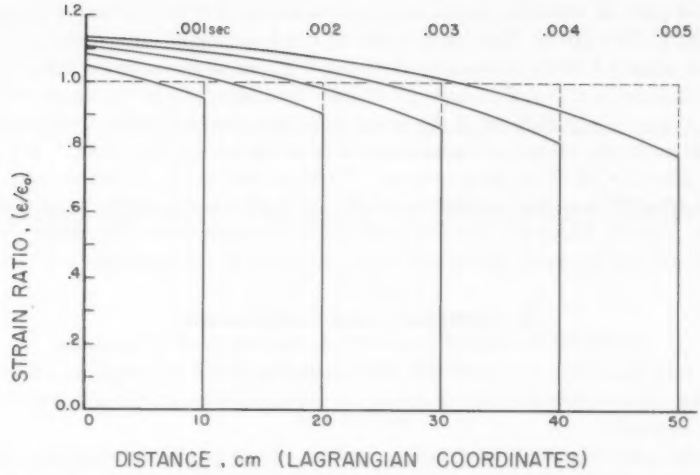

FIGURE 6. *Distribution of strain along the string for times of 1, 2, 3, 4, and 5×10^{-3} s after transverse impact.*

Calculation parameters are $\lambda = 0.2$, $m = 100$ gm^{-1}, $c = 100$ ms^{-1}, $\tau = 0.002$ s, and $V = 50$ ms^{-1}. Dash lines give distributions for an elastic string ($\lambda = 0$). The strain is expressed as the ratio of the strain ϵ at distance x to the strain ϵ_0 attained at the instant of impact.

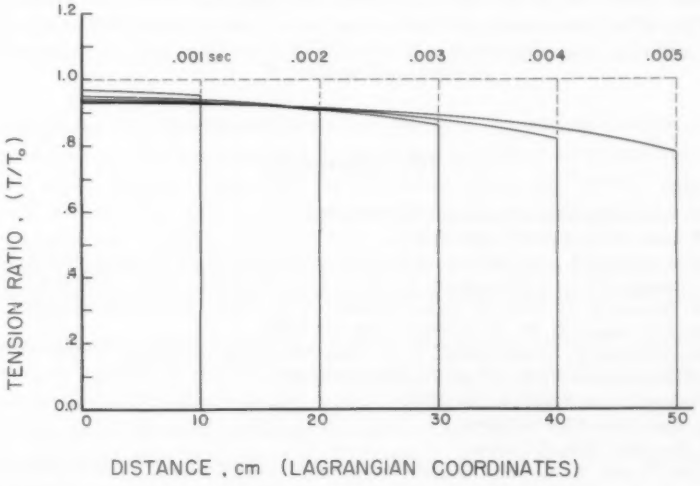

FIGURE 7. *Distribution of tension along the string for times of 1, 2, 3, 4, and 5×10^{-3} s after transverse impact.*

Calculation parameters are $\lambda = 0.2$, $m = 100$ gm^{-1}, $c = 100$ ms^{-1}, $\tau = 0.002$ s, and $V = 50$ ms^{-1}. Dash lines give distributions for an elastic string ($\lambda = 0$). The tension is expressed as the ratio of the tension T at distance x to the tension T_0 attained at the instant of impact.

attained in the case of longitudinal impact [10]. The tension distributions at various times after impact are depicted in figure 7. These distributions also are similar to those resulting from longitudinal impact at constant velocity. The tension at the point of impact decreases with time and approaches a limiting value which is less than the value of $T_0(1-\lambda)^{1/2} = 0.894T_0$ attained in the case of longitudinal impact.

The values of particle velocity, strain, and tension attained at the instant of impact are -27.50 ms^{-1}, 0.2750, and 2.750×10^2 N. The initial value of the Lagrangian transverse wave front velocity is 46.44 ms^{-1} but after 5×10^{-3}s it slows to 44.00 ms^{-1}. To an observer in the laboratory (x', y' system) the initial velocity is $(1+\epsilon_0)P_0+w_0=31.71$ ms^{-1} and after 5×10^{-3}s the wave front has traveled a distance $x'=x+\xi=0.1525$ m. If the wave front had traveled at the initial velocity, it would have gone 0.1586 m. At the instant of impact the slope of the transverse wave, $\tan\theta=\beta/\alpha$, is equal to -1.577, but after 5×10^{-3}s it decreases to -1.646 at the point of impact and -1.627 at the transverse wave front. Thus, the wave slows down as it propagates and gets slightly steeper and becomes slightly curved. However, for this calculated example these secondary coupling effects are small and would not be easily discerned by an observer in the laboratory.

9. Summary and Conclusions

This paper has described two methods for calculating wave propagation effects in a linearly viscoelastic string subjected to transverse impact at constant velocity. Results have been presented for a calculated example.

Viscoelasticity exerts both primary and secondary effects on the distributions of stress, strain, and particle or flow velocity along the string that result from constant-velocity transverse impact. The distributions resulting from the primary effect are the same as those resulting from a longitudinal impact at constant velocity, in which the strain increases, the tension decreases, and the particle velocity stays constant at the point of impact. In the secondary or coupling effect viscoelastic relaxation causes the particle velocity at the point of impact to increase with time, and associated changes to occur in the strain, tension, and particle velocity distributions.

The secondary effect also causes the transverse wave front to propagate at a gradually decreasing velocity. In addition, the transverse wave profile gets steeper and becomes gradually curved.

10. References

[1] Cristescu, N., Archiwum Mechaniki Stosowanej **12,** 597 (1960).
[2] Cristescu, N., J. Mech. Phys. Solids **9,** 165 (1961).
[3] Smith, J. C., McCrackin, F. L., and Schiefer, H. F., J. Res. NBS **60,** 517 (1958); Textile Res. J. **28,** 288 (1958).
[4] Schultz, A. B., Tuschak, P. A., and Vicario, A. A., Jr., J. Appl. Mech. **34,** Trans. ASME **89,** Series E, 392 (1967).
[5] Petterson, D. R., Stewart, G. M., Odell, F. A., and Mayheux, R. C., Textile Res. J. **30,** 411 (1960).
[6] Petterson, D. R., and Stewart, G. M., Textile Res. J. **30,** 422 (1960).
[7] Smith, J. C., Fenstermaker, C. A., and Shouse, P. J., Textile Res. J. **35,** 743 (1965).
[8] Smith, J. C., and Fenstermaker, C. A., J. Appl. Phys. **38,** 4218 (1967).
[9] Morrison, J. A., Quart. Appl. Math. **14,** 153 (1956).
[10] Smith, J. C., J. Appl. Phys. **37,** 1697 (1966).
[11] Smith, J. C., J. Res. NBS **70B,** 257 (1966).
[12] Truesdell, C., and Toupin, R. A., The Classical Field Theories. Encyclopedia of Physics, edited by S. Flugge, Vol. **III/1.** (Springer-Verlag, 1960).
[13] Fong, J. T., Ph. D. Thesis, Stanford University (1966).
[14] Jeffrey, A., and Taniuti, T., Non-linear Wave Propagation with Applications to Physics and Magnetohydrodynamics (Academic Press, 1964).

(Paper 72B3–270)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 3, July—September 1968

Allocating Service Periods to Minimize Delay Time*

W. A. Horn

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(May 28, 1968)

Consider a facility which must divide its services, during the time interval $[0, T]$, among N streams of arrivals. The problem treated is that of finding a pattern of service which minimizes total delay to the members of the streams, taking into account the "dead time" which begins each service period. For each stream, it is required that final queue size equal initial size, and that the queue be empty sometime in $[0, T]$. Conditions for feasibility of solutions are given in the case where the instantaneous service rates are bounded above by known constants. In the event that all streams have constant arrival rates and are to be served the same number of times, an optimal service pattern is derived using a recent result of R. Rangarajan and R. M. Oliver.

Key Words: Allocation; queueing theory; scheduling; switching theory; traffic flow; transportation theory.

1. Problem Statement

This paper presents a further investigation into the type of problem studied in a recent paper by Rangarajan and Oliver.[1] The problem pertains to the allocation of servicing times among several incoming streams which require "processing" of some kind by a single "server" capable of handling only one stream at a time. The server might for example be a switching point or a congestion point (e.g., a tunnel entrance) in a transport network, in which case "serving" a stream simply means permitting passage to its flow. Or, the server might be a computer handling reservations being arranged at several points, or exercising control on a real-time basis over operations along several links.

The time period during which servicing occurs is assumed to be $[0, T]$, where $T > 0$. The rate at which "customers" arrive at stream i is assumed to be the known continuous function $a_i(t)$, while the outflow or service-rate function $s_i(t)$, which will be defined below, is bounded above by the constant $C_i > 0$, the capacity when servicing stream i. It is further assumed that $a_i(t)$ crosses the level C_i at most a finite number of times in $[0, T]$. That is, $a_i^{-1}(C_i)$ is a set with a finite number of connected components.

The size of the waiting queue in stream i at time t is designated by $Q_i(t)$, and we let $q_i = Q_i(0)$, where it is assumed that each q_i is nonnegative. Then clearly

$$Q_i(t) = q_i + \int_0^t (a_i(\tau) - s_i(\tau))\,d\tau. \tag{1}$$

A cumulative waiting time function $W_i(t)$ is defined for each i by

$$W_i(t) = \int_0^t Q_i(\tau)\,d\tau,$$

*Supported by Northeast Corridor Transportation Project, Department of Transportation. No official endorsement is implied.

[1] R. Rangarajan and R. M. Oliver, Allocations of servicing periods that minimize average delay for N time-shared traffic streams, Transportation Science 1, 74–80 (1967).

and a total waiting time function $W(t)$ is defined by

$$W(t)=\sum_{i=1}^{N} W_i(t),$$

where N is the number of streams.

Since $s_i(t)$ will depend on the times at which servicing actually occurs, it is clear that W_i and W also depend on these variables. Furthermore, W_i and W depend on the quantities q_i. These functional dependencies may be expressed explicitly when convenient.

Next we define $s_i(t)$. As a preliminary, we further limit the generality of the problem by assuming that a given stream i is serviced, within $[0, T]$, only during a finite set of closed intervals $\{[x_{ij}, y_{ij}]\}_{j=1}^{m(i)}$ where $m(i)$ is the total number of such intervals of service to stream i. No two intervals of servicing, for any streams, may overlap except at their endpoints, and the set of all service intervals for all streams covers $[0, T]$. (The endpoints of these intervals comprise the *switching pattern*.) Furthermore, for some set of positive constants $\{d_i\}$ called the "dead" times, it is assumed that $x_{ij}+d_i \leq y_{ij}$, for $i=1, 2, \ldots, N$, and $j=1, 2, \ldots, m(i)$.

If stream i is not being serviced at time t, then $s_i(t)$ is defined to be 0. If t lies in the service interval $[x_{ij}, y_{ij}]$, then $s_i(t)$ is defined by

$$s_i(t)=\begin{cases}0\colon\ t\in[x_{ij},\ x_{ij}+d_i],\\ C_i\colon\ t\in(x_{ij}+d_i,\ y_{ij}] \text{ and } Q_i(t)>0,\\ \min\ (C_i,\ a_i(t))\colon\ t\in(x_{ij}+d_i,\ y_{ij}] \text{ and } Q_i(t)\leq 0.\end{cases}$$

Now it is clear from (1) that Q_i depends on s_i, whereas the above definition states that s_i depends on Q_i, at least on the intervals $(x_{ij}+d_i,\ y_{ij}]$. Thus it is necessary to show that there exist unique functions s_i and Q_i which satisfy (1) and the equation for s_i. This will be detailed in appendix A.

The above definition of s_i, together with the fact that $q_i \geq 0$, assures that $Q_i(t) \geq 0$ for all $t\in[0,T]$, since if $Q_i(t)<0$ for some t then there would exist $t'<t$ such that $Q_i(t')=0$, by the continuity of Q_i. Let t_0' be the greatest such t'. Then $Q_i(r)\leq 0$ for all r such that $t_0'\leq r\leq t$, and so $a_i(r)-s_i(r)\geq 0$ in this interval, by the definition of s_i. This contradicts the fact that

$$0>Q_i(t)=Q_i(t_0')+\int_{t_0'}^{t}(a_i(r)-s_i(r))dr.$$

The general problem to be considered is that of finding a finite set of intervals $[x_{ij}, y_{ij}]$ of service, as defined and restricted above, such that the total waiting time $W(T)$ is a minimum, given the initial values q_i.

We will consider a variant of the general problem in this paper by introducing the restrictions (for $i=1, 2, \ldots, N$)

$$q_i=Q_i(0)=Q_i(T), \tag{2}$$

$$Q_i(t)=0 \text{ for some } t\in[0, T], \tag{3}$$

and by allowing the minimization not only over the intervals of servicing but also over the parameters q_i as well. That is, the q_i will not be considered fixed but variable, subject to (2) and (3). Constraints (2) and (3) are called the *feasibility constraints*, and a solution is *feasible* if it satisfies them.

Imposing constraint (2) has the property of making the problem *periodic*, in the following sense. If we suppose that a_i is defined for all $t\geq 0$, rather than for $t\in[0, T]$, with $a_i(t+T)=a_i(t)$, and that the switching pattern is extended in such a way that stream i is being serviced at time $t+T$ if and only if it is also being serviced at time t, then $Q_i(0)=Q_i(T)$ implies

$$Q_i(t+T)=Q_i(t).$$

It is also seen from this that

$$W_i(T+t)-W_i(t)=W_i(T),$$

or,

$$W_i(nT+\theta)=nW_i(T)+W_i(\theta).$$

This in turn implies that

$$W(t)/t \to W(T)/T \text{ as } t \to \infty,$$

so that, in a sense, minimizing $W(T)$ and thus $W(T)/T$ is equivalent to minimizing the "long-term average delay." The motivation for this restriction is that the applications we have in mind refer to ongoing systems rather than isolated occurrences. It seems of little practical use (except for emergency evacuation operations and the like) to formulate the problem as if what happened after time T were of no concern. Condition (2), at least for periodic arrival patterns, implies stability in the sense of "repeatability" for the situation, in particular ruling out unbounded growth of queues over the long run. It might prove worthwhile to investigate the problem variant in which (2) is replaced by

$$Q_i(T) \leq Q_i(0), \tag{2'}$$

but this version will not be studied here.

2. Feasibility and Consistency Conditions

So far it is not known whether there exist feasible solutions of the problem of section 1. This section will be devoted to finding necessary and sufficient conditions for the existence of such solutions.

Since we are considering the problem where not only the points of switching are allowed to vary, but also the q_i, the first question which arises is how much freedom the q_i have, for a given switching pattern, so that conditions (2) and (3) may still be satisfied. The following two lemmas answer this.

LEMMA 1. *Let* Q_i *and* Q_i' *be the queue-size functions associated with the initial values* q_i *and* q_i', *respectively, and having the same switching pattern. Then* $|Q_i(t)-Q_i'(t)|$ *is a nonincreasing function of* t.

PROOF. First, Q_i-Q_i' does not change sign. For if $Q_i(a)-Q_i'(a)>0$ and $Q_i(b)-Q_i'(b)<0$, where $a<b$, then by continuity $Q_i(t)=Q_i'(t)$ for some $t\epsilon(a, b)$. But then $Q_i(\tau)=Q_i'(\tau)$ for all $\tau \geq t$, contradicting $Q_i(b)<Q_i'(b)$.

Now suppose (say) $Q_i(0)>Q_i'(0)$. Then $Q_i(t)-Q_i'(t)=|Q_i(t)-Q'(t)|$, by the above. But $Q_i(t)-Q_i'(t)=q_i-q_i'+\int_0^t (s_i'(\tau)-s_i(\tau))d\tau$, and since $s_i'(\tau) \leq s_i(\tau)$ for all $\tau\epsilon[0, T]$ because $Q_i \geq Q_i'$, we have that $|Q_i(t)-Q_i'(t)|$ is nonincreasing. Similarly if $Q_i(0)<Q_i'(0)$ or $Q_i(0)=Q_i'(0)$.

LEMMA 2. *Let* Q_i *and* Q_i' *be two queue-size functions associated with the same switching pattern during* [0, T] *and both satisfying* (2). *Then* Q_i *and* Q_i' *differ by a constant. Hence there exists at most one feasible solution for each switching pattern.*

PROOF. From lemma 1,

$$|Q_i(0)-Q_i'(0)| \geq |Q_i(t)-Q_i'(t)| \geq |Q_i(T)-Q_i'(T)|$$

for all $t\epsilon[0, T]$. But by (2), $|Q_i(0) - Q_i'(0)| = Q_i(T) - Q_i'(T)|$. Hence, by the continuity of the queue-size functions, $Q_i(t) - Q_i'(t) = q_i - q_i'$, a constant.

Now if two solutions having the same switching pattern are both feasible, then they satisfy (3) in addition to (2). But if $q_i > q_i'$, for example, then $Q_i(t) > Q_i'(t) \geq 0$, by the above, and Q_i is not feasible. Therefore $q_i = q_i'$ and so $Q_i = Q_i'$.

The next question to be treated is which patterns of switching times admit feasible solutions.

THEOREM 3. *Suppose that stream* i *is serviced during successive intervals of length*

$$L_{i1}, L_{i2}, \ldots, L_{im(i)},$$

and let d_i *be the dead time for stream* i. *Then a necessary and sufficient condition that a set of* q_i *exist for which the given switching pattern produces a feasible solution is*

$$C_i \sum_{j=1}^{m(i)} L_{ij} \geq \int_0^T a_i(t)dt + m(i)C_i d_i$$

for all i.

PROOF. Let the above inequality be satisfied. It is clear that, when q_i is sufficiently large, $Q_i(t) > 0$ for all $t\epsilon[0, T]$. Then, by definition, $s_i(t) = 0$ during nonservice intervals and during a part d_i of each service interval, and $s_i(t) = C_i$ otherwise. Thus for such q_i,

$$\int_0^T s_i(t)dt = C_i \sum_{j=1}^{m(i)} (L_{ij} - d_i) = C_i \sum_{j=1}^{m(i)} L_{ij} - C_i m(i) d_i \geq \int_0^T a_i(t)dt,$$

so that

$$Q_i(T) = q_i + \int_0^T (a_i(t) - s_i(t))dt \leq q_i.$$

On the other hand, for $q_i = 0$ it is clear that $Q_i(T) \geq q_i$. But for a fixed switching pattern, $Q_i(T)$ is a continuous function of q_i. (In fact, by lemma 1, $|Q_i(T) - Q_i'(T)| \leq |q_i - q_i'|$.) Thus there exists a q_i for which $Q_i(T) = q_i$.

Let q_i^0 be the infimum of all such q_i satisfying $q_i = Q_i(T)$ for the given pattern of switching. Let

$$b = \inf \{Q_i(t) : t\epsilon[0, t], Q_i(0) = q_i^0\}.$$

If $b = 0$, then q_i^0 gives a feasible solution. But if $b > 0$, then using the value $q_i = q_i^0 - b/2$ as the initial queue size, we find that $Q_i(t) \geq b - b/2 = b/2$ for all $t\epsilon[0, T]$, by lemma 1. Thus by the definition of s_i we have the same value of $s_i(t)$, for each $t\epsilon[0, T]$, for the two initial values q_i^0 and $q_i^0 - b/2$. But this implies that the solution with initial value $q_i^0 - b/2$ also satisfies (2), contradicting the definition of q_i^0.

This proves sufficiency. Necessity follows from (2), noting that

$$\int_0^T a_i(t)dt = \int_0^T s_i(t)dt \leq C_i \sum_{j=1}^{m(i)} (L_{ij} - d_i).$$

LEMMA 4. *Suppose there exist numbers* $T_i > 0$ *such that*

$$\sum_{i=1}^{N} T_i = T$$

and

$$C_i T_i \geq \int_0^T a_i(t)dt + m(i)C_i d_i.$$

Then there exists a feasible solution for which stream i *is serviced exactly* m(i) *times (some of which may be consecutive), and there exists an optimal such solution relative to the particular* m(i)*'s.*

PROOF. By Theorem 3, if $\{L_{ij}\}$ is a set satisfying

$$\sum_{j=1}^{m(i)} L_{ij} = T_i,$$

where each $L_{ij} \geq d_i$, then L_{ij} represents a feasible solution. By lemma 2, q_i is uniquely determined by the switching pattern. But the vector of switching times is a point of

$$[0, T]^{\Sigma m(i)},$$

a compact set. The conditions (given in Lemma 2) defining those switching patterns which correspond to feasible solutions are linear inequalities in the L_{ij}'s, and so in the switching times themselves; thus the minimization is to take place over a closed subset of the compact set.

It will be shown in appendix B that $W(T)$ is continuous in the vector of switching times. Since this in turn ranges over a compact set, an optimal solution must exist.

The last result permits us to state explicit conditions for the existence of an optimal solution in the simplest case, namely for constant a_i.

COROLLARY 5. *Suppose* $a_i(t) = a_i$, *a constant. If* $\{L_{ij}\}$ *are the service interval lengths of a switching pattern such that*

$$\sum_{j=1}^{m(i)} L_{ij} \geq m(i)d_i + a_i T/C_i, \tag{4}$$

then the pattern is feasible. Furthermore, if numbers $T_i > 0$ *exist such that*

$$\sum_{i=1}^{N} T_i = T$$

and

$$T_i \geq m(i)d_i + a_i T/C_i,$$

then an optimal feasible solution exists.

PROOF. From Theorem 3 and Lemma 4.

Now let $\rho_i = a_i/C_i$ and $d = \sum_{i=1}^{N} m(i)d_i$. Then we have the following.

THEOREM 6. *For constant* a_i, *the following conditions are necessary and sufficient for the existence of a feasible solution with* m(i) *servicings of stream* i *which is optimal with respect to the given set* {m(i)}:

$$\sum_{i=1}^{N} \rho_i < 1, \tag{5}$$

$$T \geq \frac{d}{1 - \sum_{i=1}^{N} \rho_i}. \tag{6}$$

PROOF. If $\{L_{ij}\}$ is feasible, by Lemma 5 it must satisfy (4). Summing (4) over all i, we get

$$T \geq \sum_{i=1}^{N} m(i)d_i + T \sum_{i=1}^{N} (a_i/C_i) = d + T \sum_{i=1}^{N} \rho_i, \tag{7}$$

or equivalently

$$T\left(1-\sum_{i=1}^{N}\rho_i\right)\geq d>0.$$

Since $T>0$, we have $1-\sum_{i=1}^{N}\rho_i>0$, proving (5), and also

$$T\geq\frac{d}{1-\sum_{i=1}^{N}\rho_i},$$

proving (6).

Now suppose (5) and (6) are satisfied. Then (7) is also satisfied. Thus it is possible to find $T_i>0$ such that

$$T_i\geq m(i)d_i+a_iT/C_i.$$

The result follows from Corollary 5.

3. Optimal Solutions for Constant Arrival Rates and Equal $m(i)$'s

This section will deal with the special case in which each $a_i(t)$ is a constant function, and the $m(i)$ are all equal to some common value m. This case was treated by Rangarajan and Oliver (see footnote 1), with the further provision that $m=1$, that is, that each stream was serviced exactly once.

A method of finding the optimum service period length for each stream was found (see footnote 1), and this is the result to be generalized here. It will be shown that an optimum (not necessarily *the* optimum) switching pattern is obtained for the case $m(i)=m$, a_i constant, when the interval $[0, T]$ is broken up into m subintervals of equal length, the switching pattern is optimized over the first interval $[0, T/m]$ by the methods of [1] with one servicing per stream, and this pattern is repeated cyclically for each of the other $m-1$ subintervals. In addition to this, an auxiliary result (see footnote 1) will be used to find the optimum value of m.

LEMMA 7. *Suppose that in the interval* [s, t] *the function* f(x) *is either increasing at a rate* p *or decreasing at a rate* $-$q *almost everywhere. Suppose that* f(s)= f(t)=0 *and that* f(x) $\geq$ 0 *for* x$\in$(s, t). *Suppose further that* f *increases during* (s, s+ A_1), *decreases during* (s+ A_1, s+ A_1 + B_1), *etc., where each interval of increase of length* A_i *is followed by an interval of decrease of length* B_i *and each interval of decrease of length* B_i *is followed by an interval of increase of length* A_{i+1}, *the last intervals being of length* A_n *and* B_n *respectively. Then*

$$\int_s^t f(x)dx\geq\frac{p(p+q)}{2q}\sum_{i=1}^{n}A_i^2.$$

PROOF. The proof is geometric in nature and is by induction on n. First, for $n=1$ the inequality reduces to

$$\int_s^t f(x)dx\geq\frac{p(p+q)}{2q}A_1^2.$$

Referring to figure 1, we see that $\int_s^t f(x)dx$ is the area of the triangle whose altitude is A_1p and whose base is A_1+B_1, where

$$B_1=A_1p/q.$$

Thus $\int_s^t f(x)dx = \frac{p(p+q)}{2q} A_1^2$, proving the case $n=1$.

Assume that the lemma has been proved for $1, 2, \ldots, n-1$. Looking at figure 2, we see that

$$\int_s^t f(x)dx \geq \frac{p(p+q)}{2q} \sum_{i=1}^{n-1} A_i^2 + \text{Area } YWVZX \geq \frac{p(p+q)}{2q} \sum_{i=1}^{n-1} A_i^2 \Delta XYZ$$

$$= \frac{p(p+q)}{2q} \sum_{i=1}^{n-1} A_i^2 + \frac{p(p+q)}{2q} A_n^2 = \frac{p(p+q)}{2q} \sum_{i=1}^{n} A_i^2.$$

We now state the following notations to be used during the rest of this section. I_{ij} will denote the jth interval of service for lane i during $[0, T]$. Because of the cyclic character of the problem we also define

$$I_{ik} \equiv I_{ij}$$

where $1 \leq j \leq m$ and $k \equiv j \pmod{m}$. We denote the length of I_{ij} by L_{ij}. The interval contained between I_{ij} and $I_{i,j+1}$ (or the two intervals, if $j=m$) will be denoted by J_{ij} and its length (respectively, the sum of their lengths) by M_{ij}.

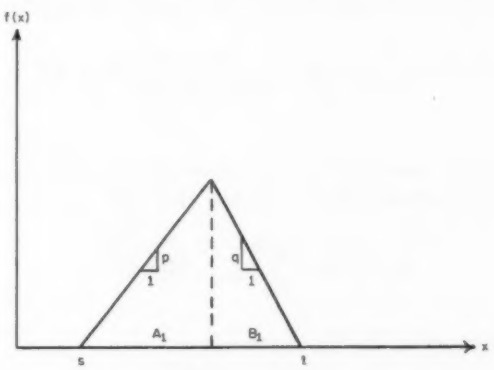

FIGURE 1.

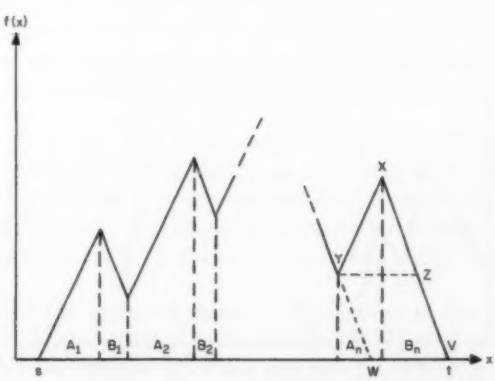

FIGURE 2.

LEMMA 8. *Let S be a feasible switching pattern for a problem with constant* a_i. *Then*

$$W_i(T) \geq \frac{a_i C_i}{2(C_i - a_i)} \sum_{j=1}^{m} (M_{ij} + d_i)^2.$$

PROOF. By definition, W_i is the integral of Q_i, which is always nonnegative. Thus W_i may be thought of as the area under the curve representing Q_i. Since $C_i > a_i$ in order to satisfy feasibility, Q_i is either rising at a rate a_i (when $s_i = 0$), falling at a rate $-(C_i - a_i)$ (when $s_i = C_i$), or constant at 0 (when $s_i = a_i$). We may represent this as in figure 3. It is also clear that the curve is rising only during the time that lane i is not being serviced, plus the dead time, that is, during intervals of length $M_{ij} + d_i$.

Now let us group the I_{ij} as follows. By condition (3), there exists $t_0 \in [0, T]$ such that $Q_i(t_0) = 0$. Let I_{ij} be the interval of service to lane i to which t_0 belongs. (Obviously t_0 must lie in some interval of service.) Let I_{ik} be the first interval after I_{ij} during which $Q_i(t)$ is again 0. Then the lengths of the intervals of nonservice to i between I_{ij} and I_{ik}, namely J_{ij}, $J_{i,j+1}$, . . . , $J_{i,k-1}$, will be M_{ij}, $M_{i,j+1}$, . . . , $M_{i,k-1}$. If we let z_{iq} represent the right endpoint of any interval I_{iq}, then from Lemma 7 we have

$$\int_{z_{ij}}^{z_{ik}} Q_i(t)\,dt \geq \frac{a_i C_i}{2(C_i - a_i)} \sum_{\nu=j}^{k-1} (M_{i\nu} + d_i)^2.$$

Summing this inequality over all intervals in which Q_i becomes 0, we get

$$W_i(T) = \int_0^T Q_i(t)\,dt \geq \frac{a_i C_i}{2(C_i - a_i)} \sum_{j=1}^{m} (M_{ij} + d_i)^2.$$

This proves the lemma.

THEOREM 9. *Suppose that, for constant* a_i, $\{I_{ij}\}$ *represents an optimal feasible solution, where* $m(i = m$. *Then there exists an optimal feasible solution* $\{\bar{I}_{ij}\}$ *with*

$$\bar{L}_{ij} = (1/m) \sum_{k=1}^{m} L_{ik}, \qquad 1 \leq i \leq n,$$

where $\bar{L}_{ij}$ *is the length of interval* $\bar{I}_{ij}$, L_{ij} *the length of* I_{ij}.

PROOF. Consider the solution defined by $\bar{L}_{ij} = (1/m) \sum_{k=1}^{m} L_{ik}$, where $\bar{I}_{1,1}$ is the first interval and

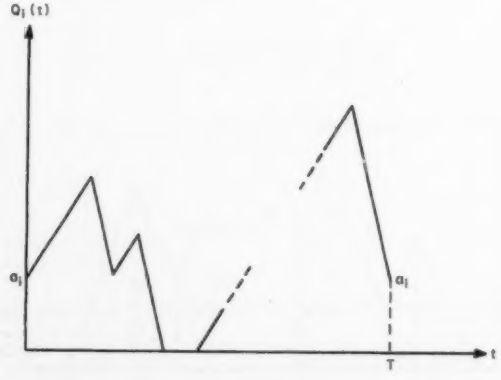

FIGURE 3.

where interval $\bar{I}_{ij}$ is followed by $\bar{I}_{i+1,j}$ for $i < n$, and interval $\bar{I}_{nj}$ is followed by $\bar{I}_{1,j+1}$. Then we have

$$\bar{M}_{ij} = \bar{M}_i, \qquad 1 \leq j \leq n.$$

By lemma 8, the waiting time for the original solution satisfies

$$\bar{W}_i(T) \geq \frac{a_i C_i}{2(C_i - a_i)} \sum_{j=1}^{m} (M_{ij} + d_i)^2,$$

and the Cauchy-Schwartz inequality yields

$$\sum_{j=1}^{m} (M_{ij} + d_i)^2 \geq m(\bar{M}_{ij} + d_i)^2 = \sum_{j=1}^{m} (\bar{M}_{ij} + d_i)^2.$$

Thus it suffices to show that the new solution (which by Corollary 5 is feasible) obeys Lemma 8 with *equality*, i.e., that

$$\bar{W}_i(T) = \int_0^T \bar{Q}_i(t)\,dt = \frac{a_i C_i}{2(C_i - a_i)} \sum_{j=1}^{m} (\bar{M}_{ij} + d_i)^2.$$

From the proofs of Lemmas 7 and 8, it should be apparent that this is equivalent to proving that $\bar{Q}_i$ is reduced to 0 during *each* service interval $\bar{I}_{ij}$. The condition for this is

$$(C_i - a_i)(\bar{L}_{ij} - d_i) \geq a_i(\bar{M}_{ij} + d_i), \tag{8}$$

which will now be demonstrated.

By corollary 5,

$$m\bar{L}_{ij} = \sum_{j=1}^{m} L_{ij} \geq md_i + a_i T/C_i,$$

and so

$$C_i(\bar{L}_{ij} - d_i) \geq a_i(T/m) = a_i(\bar{M}_{ij} + d_i + (\bar{L}_{ij} - d_i)),$$

implying (8) as desired.

Note that Theorem 9 merely establishes the form of one optimal solution. It is clear that we could get a set of optimal solutions by permuting indices. Furthermore, it could probably be shown that these solutions are the only ones which are optimal, but this would involve solving a set of simultaneous linear equations relating the M_{ij} and L_{ij} and this is not considered here to be worth the trouble.

Also, nothing is said about the case where $m(i) \neq m(k)$. This seems to be a much harder case to analyze generally. However, if $N = 2$ the above proof may be modified so that this problem is completely solved. For in that case it is obvious that $m(1) = m(2)$, since otherwise two servicings of some lane would be consecutive, giving a higher value for $\bar{W}$ than that obtained by merging the two consecutive servicings into one. Also, $L_{1j} = M_{2,j-1}$ and $L_{2j} = M_{1j}$. Thus the condition $M_{ij} = M_{ik}$ is equivalent to $L_{ij} = L_{ik}$.

Finally, we shall discuss the optimum value of m to choose in the above problem, given T. Note that if $\{I_{ij}\}$ denotes an optimal solution on the interval $[0, T]$ as described above, where each lane is serviced once during the interval $[0, T/m]$ and this procedure is repeated m times, then we have

312-532 O - 68 - 5

$$mW(T/m) = W(T).$$

This recalls the work of Rangarajan and Oliver (see footnote 1) in which the function to be minimized is $W(T)/T$ instead of $W(T)$. (Of course, for constant T, minimizing $W(T)$ is equivalent to minimizing $W(T)/T$, and the first part (see footnote 1) considers the problem in this way.) We show how the results can be applied to the above problem.

Suppose that T' is a variable which is allowed to take on only the discrete set of values T/m, m an integer, in the problem where each lane is serviced exactly once during the interval $[0, T']$. If $W(T')/T'$ attains its minimum value on this discrete set at the point $T' = T'_0 = T/m_0$, then $W(T)$ in the original problem attains its minimum value over all m for $m = m_0$. For we have

$$\frac{W(T/m_0)}{T/m_0} \leq \frac{W(T/m)}{T/m},$$

for $m \neq m_0$; or,

$$m_0 W(T/m_0) \leq mW(T/m).$$

But by the above remarks, $mW(T/m) = W(T)$ where $W(T)$ is calculated for m cycles of service in the interval $[0, T]$, and similarly for $m_0 W(T/m_0)$.

Thus it is clear that finding m_0 such that $W(T)$, optimized over all switching patterns, attains its least value when each stream is serviced m_0 times, is equivalent to finding m_0 such that $W(T/m_0)/(T/m_0)$ is a minimum for the optimized solution of the one-cycle case. Now a method is given (see footnote 1) to optimize $W(T')/T'$ when T' is a continuous variable, and it is shown that $W(T')/T'$ is monotone decreasing to the left of the optimum, $T' = T'_0$, and monotone increasing to the right. Thus if n is an integer such that

$$T/(n+1) \leq T'_0 \leq T/n,$$

it is clear that the optimum value m_0 sought above must be either n or $n+1$. In order to determine which of these values is optimum, it is only necessary to substitute in the expression for the optimized value of $W(T')/T'$, also given (see footnote 1). Thus m_0 is easily determined.

4. Appendix A: Uniqueness of Q_i

We show here that the s_i, and hence the Q_i, are well defined by the definition given in the text. First, it is clear that $s_i(t) = 0$ when t is not in some interval of the form $(x_{ij} + d_i, y_{ij})$. Let us divide each interval $(x_{ij} + d_i, y_{ij})$ into subintervals in which either $a_i(t) > C_i$ or $a_i(t) \leq C_i$ for all t in the subinterval. It is clear that there will be a finite number of such subintervals, since $a_i(t)$ crosses the value C_i at most a finite number of times.

In the subintervals where $a_i(t) > C_i$, it is clear that $a_i(t) - s_i(t) > 0$, so that $Q_i(t) > 0$ and hence we must have $s_i(t) = C_i$.

Now assume that $[b, c]$ is a subinterval such that $a_i(t) \leq C_i$ for $t \in [b, c]$, and that Q_i has been defined for $t \in [0, b]$. Let

$$\overline{Q}_i(t) = Q_i(b) + \int_b^t (a_i(\tau) - C_i)\, d\tau,$$

and $Q_i(t) = \max(\overline{Q}_i(t), 0)$, for $t \in [b, c]$. We will show that this gives the only possible value for Q_i.

For if $\bar{Q}_i(t) > 0$ for some $t\epsilon[b, c]$, then since Q_i is changing in $[b, t]$ at a rate at least as great as $a_i(\tau) - C_i$, it is clear that $Q_i \geq \bar{Q}_i$. Thus, $s_i(t) = C_i$ for such t and so $Q_i = \bar{Q}_i$. Now if $\bar{Q}_i(t) \leq 0$ for some $t\epsilon[b, c]$, since $\bar{Q}_i$ is continuous we can find a first point τ in $[b, c]$ where $\bar{Q}_i(\tau) = 0$. By the above argument, $Q_i(\tau) = 0$ also. Since $s_i(t) \geq a_i(t)$ in the interval $[b, c]$, we must then have that $Q_i(t) \leq 0$ for all $t\epsilon[\tau, c]$, by the definition of Q_i, and so $Q_i(t) = 0$, satisfying the above assertion.

5. Appendix B: Continuity of the Objective Function

We next show that the value $W(T)$ associated with a feasible solution defined by a given switching pattern

$$\{[x_{ij}, y_{ij}]\}$$

is uniformly continuous in the x_{ij} and y_{ij}. Let $\{[x_{ij}, y_{ij}]\}$ and $\{[x'_{ij}, y'_{ij}]\}$ be two switching patterns such that, for some stream r, the service intervals for stream r are exactly the same in both patterns except for one interval endpoint, say x_{rp}. Let Q_r and Q'_r be the respective queue-size functions for stream r associated with $\{[x_{ij}, y_{ij}]\}$ and $\{[x'_{ij}, y'_{ij}]\}$. Suppose that $x'_{rp} < x_{rp}$, so that stream r is serviced more by the second pattern. Let $q_r = Q_r(0)$ and $q'_r = Q'_r(0)$.

Construct a new queue-size function $\bar{Q}_r$ as the (possibly not feasible) function associated with initial size q_r and switching pattern $\{[x'_{ij}, y'_{ij}]\}$. It is clear, by the previous section, that

$$\bar{Q}_r(t) = Q_r(t)$$

for $t\epsilon[0, x'_{rp}]$. Also, since

$$s_r(t) \geq \bar{s}_r(t)$$

for $t\epsilon[x'_{rp}, x_{rp}]$, where s_r and $\bar{s}_r$ are the service-rate functions of the two patterns, we have

$$\bar{Q}_r(t) \leq Q_r(t)$$

for $t\epsilon[x'_{rp}, x_{rp}]$, and hence $\bar{Q}_r(x_{rp}) \leq Q_r(x_{rp})$. Since the two patterns are the same for the rest of the interval, $[x_{rp}, T]$, we have by lemma 1 that

$$\bar{Q}_r(t) \leq Q_r(t)$$

for $t\epsilon[x_{rp}, T]$.

Let $\bar{\bar{Q}}_r$ be the queue-size function defined by

$$\bar{\bar{Q}}_r(0) = \bar{q}_r = \bar{Q}_r(T)$$

and having a switching pattern $\{[x'_{ij}, y'_{ij}]\}$. Since $Q_r(t)$ represents a feasible solution, there exists $\tau\epsilon[0, T]$ such that $Q_r(\tau) = 0$. But then

$$\bar{Q}_r(\tau) \leq Q_r(\tau) = 0,$$

implying $\bar{Q}_r(\tau) = 0$. Now $\bar{\bar{Q}}_r$ has the same switching pattern as $\bar{Q}_r$, and

$$\bar{q}_r = \bar{Q}_r(T) \leq Q_r(T) = q_r,$$

so that $\bar{\bar{Q}}_r(t) \leq \bar{Q}_r(t)$ for all $t\epsilon[0, T]$, and hence

$$\bar{\bar{Q}}_r(\tau) \leq \bar{Q}_r(\tau) = 0,$$

implying $\overline{\overline{Q}}_r(\tau)=0$. Since $\overline{\overline{Q}}_r$ and $\overline{Q}_r$ have the same switching pattern we may then conclude that

$$\overline{\overline{Q}}_r(t)=\overline{Q}_r(t)$$

for $t\epsilon[\tau, T]$, and so

$$\overline{\overline{Q}}_r(T)=\overline{Q}_r(T)=\bar{q}_r.$$

Thus $\overline{\overline{Q}}_r$ is feasible and so $Q'_r=\overline{\overline{Q}}_r$, by lemma 2.

But $\{[x_{ij}, y_{ij}]\}$ and $\{[x'_{ij}, y_{ij}]\}$ differ only on the portion (x'_{rp}, x_{rp}), as far as stream r is concerned, and so Q_r and Q'_r may differ by at most

$$C_r(x_{rp}-x'_{rp})$$

by the above and by Lemma 1.

Now consider any two feasible switching patterns $\{[x_{ij}, y_{ij}]\}$ and $\{[x'_{ij}, y'_{ij}]\}$, and let δ_i be the shortest distance between successive intervals of service to the ith stream in either pattern. That is,

$$\delta_i=\min\{\min_j(x_{i,j+1}-y_{ij}), \min_j(x'_{i,j+1}-y'_{ij})\}.$$

If we have $|x_{ij}-x'_{ij}|<\delta_i/3$ and $|y_{ij}-y'_{ij}|<\delta_i/3$ for all j, then

$$|Q_i(t)-Q'_i(t)|\leq C_i\sum_j(|x_{ij}-x'_{ij}|+|y_{ij}-y'_{ij}|).$$

For we may find a sequence of feasible switching patterns connecting $\{[x_{ij}, y_{ij}]\}$ and $[\{x'_{ij}, y'_{ij}]\}$ such that each two adjacent patterns of the sequence differ in only one coordinate. This is done by first changing the x_{ij} to x'_{ij} and the y_{ij} to y'_{ij} so that at each step the interval length L_{ij} is increased. When no more such changes are possible, the remaining x_{ij} are changed to x'_{ij} and the remaining y_{ij} to y'_{ij}. Since the sum of interval lengths is not decreased below the smaller of the sum of interval lengths for the primed and the unprimed patterns during this process, and since no intervals overlap during the process (because changes in endpoints are smaller than $\delta_i/3$), all switching patterns in the sequence are feasible.

Finally, for *any* two switching patterns $\{[x_{ij}, y_{ij}]\}$ and $\{[x'_{ij}, y'_{ij}]\}$ we assert that

$$|Q_i(t)-Q'_i(t)|\leq C_i\sum_j(|x_{ij}-x'_{ij}|+|y_{ij}-y'_{ij}|).$$

For it is possible to find a set of intermediate switching patterns

$$\{[x^0_{ij}, y^0_{ij}]\}, \{[x^1_{ij}, y^1_{ij}]\}, \ldots \{[x^m_{ij}, y^m_{ij}]\}$$

connecting $\{[x_{ij}, y_{ij}]\}$ and $\{[x'_{ij}, y'_{ij}]\}$ whose interval separations are all at least as great as the smallest interval separation, δ_i, of the given pair of patterns. This is done merely by defining

$$x^k_{ij}=\frac{k}{m}x_{ij}+\frac{m-k}{m}x'_{ij},$$

$$y_{ij}^k = \frac{k}{m} y_{ij} + \frac{m-k}{m} y'_{ij}.$$

If m is chosen large enough, then we also have that

$$|x_{ij}^k - x_{ij}^{k+1}| < \delta_i/3, \qquad |y_{ij}^k - y_{ij}^{k+1}| < \delta_i/3,$$

so that the above inequality for $|Q_i - Q_i'|$ follows easily.

This proves uniform continuity of the Q_i in the switching pattern. A proof of the continuity of $W(T)$ in the switching pattern follows from elementary calculus.

(Paper 72B3–271)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 3, July–September 1968

The Second Orthogonality Conditions in the Theory of Proper and Improper Rotations. I. Derivation of the Conditions and of Their Main Consequences*

Harry Gelman

The MITRE Corporation, Bedford, Massachusetts 01730

(June 19, 1968)

A new set of orthogonality conditions is derived for real three-by-three orthogonal matrices which describe transformations in Euclidean three-dimensional space. The principal consequences of these conditions are obtained. These are: (1) the existence and construction of the intrinsic vector of the transformation, (2) an equation connecting the trace of a transformation matrix with that of its square, which, for rotations, can be solved to give the well-known trace formula analytically, (3) a simple formula for the determinant of a transformation matrix directly in terms of the relative handedness of the two coordinate systems connected by the transformation, (4) the secular equation for a transformation matrix.

Key Words: Matrices; orthogonal transformations; rotation.

1. Introduction

There are several ways to represent proper and improper rotations in three-dimensional space. They can be represented by dyadics, which are linear operators on the vectors of Euclidean three-dimensional space [1].[1] Quaternions offer a more abstract and more elegant means of representation [2]. The quaternion representation leads to, and is equivalent to, a representation in terms of the group $SU(2)$ of two-dimensional unitary matrices with determinant unity [3]. The simplest representation to work with, and by means of which to visualize proper and improper rotations, is in terms of real, three-by-three orthogonal matrices [4]. This is the representation which we will be concerned with in this series of papers. In this series of papers the word "transformation," will generically denote the kind of transformation which is described by a general, real, three-by-three, orthogonal matrix, without regard to the value of the determinant of the matrix. When it is necessary to take the value of the determinant into account we will speak of the transformations with determinant plus one as "rigid rotations," or "proper rotations," or simply "rotations," and the transformations with determinant minus one as "improper rotations."

The usual definition of orthogonality of the underlying coordinate systems in three-dimensional Euclidean space, leads to a well-known set of conditions on the elements of the transformation matrices. We will refer to these conditions [eqs (7)] as the first orthogonality conditions. The properties of the matrices cannot, however, be deduced directly from these conditions. Instead, specific properties must be deduced analytically or geometrically. For example, the axis of a proper rotation is usually found from Euler's theorem [5], while the angle of rotation may be found by considering the action of the rotation matrix on specific vectors.

*An invited paper. This work was supported by the Electronic Systems Division of the United States Air Force under contract No. AF19(628)-5165, Project 4966.
[1] Figures in brackets indicate the literature references at the end of this paper.

By considering an alternative but equivalent definition of orthogonality of the underlying coordinate systems, it is possible to derive a new set of orthogonality conditions on the transformation matrices. We will refer to these new conditions as the second orthogonality conditions [eqs (9)]. They have the important quality of being working relations. From them, one can deduce, for example, all of the well-known properties of rotation matrices, in most cases more elegantly and concisely than with the usual methods of deducing these properties. One can also deduce some new properties.

The purpose of this paper is to derive the second orthogonality conditions (sec. 2), and to deduce their main consequences (sec. 3). Discussion of some of the consequences will be presented in subsequent papers in this series. It is hoped that the series as a whole offers a unified and simple presentation of the theory of proper and improper rotations which will be practically and pedagogically useful.

As is well known, transformations can be regarded as either passive or active. In a passive transformation all physical objects are regarded as being fixed in space while the transformations are carried out on coordinate systems. In an active transformation, there is a single coordinate system which is thought of as being unaffected, while the transformations act on physical objects in space. Although the two interpretations are equivalent for the purposes of this series of papers, it is nevertheless useful in visualizing transformations, to favor one interpretation. For the most part we will regard them as passive transformations.

2. The Second Orthogonality Conditions

We consider the transformation between a Cartesian coordinate system S, whose axes are specified by a triad of mutually orthogonal unit vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, and a system S' which is cooriginal with S, specified by the triad $\mathbf{b}'_1$, $\mathbf{b}'_2$, $\mathbf{b}'_3$. In this transformation, which is illustrated in figures 1, we take into account the possibility that the handedness of S' might differ from that of S. The customary way to express the unit normalization and mutual orthogonality of the vectors in each triad is by means of the relations

$$\mathbf{b}_i \cdot \mathbf{b}_j = \delta_{ij}, \tag{1a}$$

$$\mathbf{b}'_i \cdot \mathbf{b}'_j = \delta_{ij}, \tag{1b}$$

where δ_{ij} is the Kronecker delta, equal to zero for $i \neq j$ and equal to one when $i = j$. There is an alternative expression of orthogonality of basis vectors of a coordinate system which has the advantage over the expressions (1) that it allows for the explicit inclusion of the handedness of the particular coordinate system. This expression of orthogonality, for the coordinate systems S and S', respectively, is [2]

$$\mathbf{b}_i \times \mathbf{b}_j = p\epsilon_{ijk}\mathbf{b}_k, \tag{2a}$$

$$\mathbf{b}'_i \times \mathbf{b}'_j = p'\epsilon_{ijk}\mathbf{b}'_k, \tag{2b}$$

where ϵ_{ijk} is the Levi-Civita symbol, which is antisymmetric in the interchange of any two of its indices (implying that it vanishes when any two of its indices are equal), and is equal to one when (i, j, k) is equal to (1, 2, 3) or to any cyclic permutation of (1, 2, 3). The factors p and p' are the "handedness" factors, which are equal to one for a right handed coordinate system, and to minus one for a left handed system. The choice of handedness that is associated with $p = +1$ is dictated by the fact that we are using the conventional right handed cross product in eqs (2).

[2] In eqs (2) and subsequently in this series of papers, we use the customary convention that a repeated index on any one side of an equation is to be summed over its range.

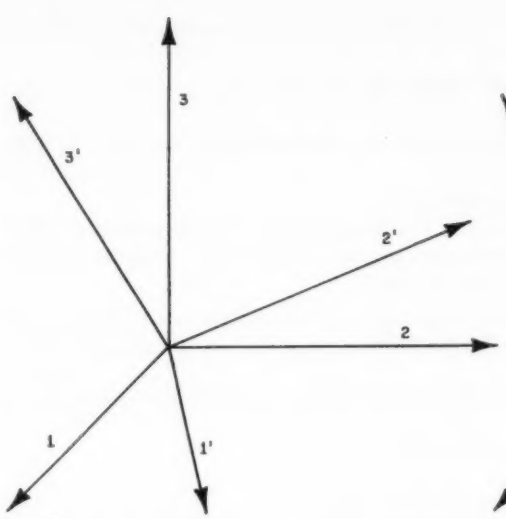

FIGURE 1a. *An orthogonal transformation which does not bring about a change of handedness.*

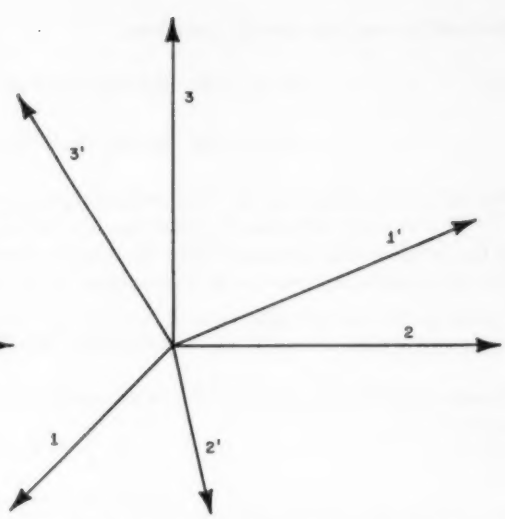

FIGURE 1b. *An orthogonal transformation which brings about a change in handedness.*

The eqs (2) as they stand do not guarantee the unit normalization of the vectors in each triad. To insure such normalization, one adds the supplementary requirements

$$\mathbf{b}_1 \cdot \mathbf{b}_2 \times \mathbf{b}_3 = p, \tag{3a}$$

$$\mathbf{b}'_1 \cdot \mathbf{b}'_2 \times \mathbf{b}'_3 = p'. \tag{3b}$$

Equations (2) and (3) immediately lead to eqs (1). In addition to being orthonormal, the $\mathbf{b}$ and $\mathbf{b}'$ triads are each separately complete. This is expressed by

$$\mathbf{b}_i \mathbf{b}_i = \mathbf{I}, \tag{4a}$$

$$\mathbf{b}'_i \mathbf{b}'_i = \mathbf{I}, \tag{4b}$$

where $\mathbf{I}$, the unit dyadic, has the property that $\mathbf{I} \cdot \mathbf{F} = \mathbf{F} \cdot \mathbf{I} = \mathbf{F}$ for any vector $\mathbf{F}$.

The matrix of transformation $A = (A_{ij})$ between S and S' is constructed from the cosines of the angles between the $\mathbf{b}$ and $\mathbf{b}'$ vectors. To be specific we define

$$A_{ij} \equiv \mathbf{b}'_i \cdot \mathbf{b}_j . \tag{5}$$

The elements of A then appear as the coefficients of expansion of the vectors of either triad in terms of the other triad as basis. These expansions are obtained by using the completeness relations (4),

$$\mathbf{b}'_i = \mathbf{b}'_i \cdot \mathbf{I} = \mathbf{b}'_i \cdot \mathbf{b}_j \mathbf{b}_j = (\mathbf{b}'_i \cdot \mathbf{b}_j)\mathbf{b}_j = A_{ij}\mathbf{b}_j, \tag{6a}$$

$$\mathbf{b}_i = \mathbf{b}_i \cdot \mathbf{I} = \mathbf{b}_i \cdot \mathbf{b}'_j \mathbf{b}'_j = (\mathbf{b}'_j \cdot \mathbf{b}_i)\mathbf{b}'_j = A_{ji}\mathbf{b}'_j. \tag{6b}$$

As a result of the orthonormality and completeness of the $\mathbf{b}$ and $\mathbf{b}'$ vectors, the matrix A satisfies

the well known orthogonality relations

$$A_{ij}A_{kj}=(\mathbf{b}'_i\cdot\mathbf{b}_j)(\mathbf{b}'_k\cdot\mathbf{b}_j)=\mathbf{b}'_i\cdot(\mathbf{b}_j\mathbf{b}_j)\cdot\mathbf{b}'_k=\mathbf{b}'_i\cdot\mathbf{b}'_k=\delta_{ik}, \tag{7a}$$

$$A_{ji}A_{jk}=(\mathbf{b}'_j\cdot\mathbf{b}_i)(\mathbf{b}'_j\cdot\mathbf{b}_k)=\mathbf{b}_i\cdot(\mathbf{b}'_j\mathbf{b}'_j)\cdot\mathbf{b}_k=\mathbf{b}_i\cdot\mathbf{b}_k=\delta_{ik}. \tag{7b}$$

We will refer to these as the first orthogonality conditions.

The second orthogonality relations are derived by [illegible]ing that the transformation of either of the cross product relations (2) by the transformations ([illegible]duces the other one of the relations (2). If eq (6a) is inserted for $\mathbf{b}'$ everywhere in eq (2b), we get

$$A_{ir}A_{jm}\mathbf{b}_r\times\mathbf{b}_m=p'\epsilon_{ijk}A_{kn}\mathbf{b}_n.$$

Equation (2a) is now used for the cross product on the left side of this equation. The result may be written

$$\left(A_{ir}A_{jm}\epsilon_{rmn}-\frac{p'}{p}\epsilon_{ijk}A_{kn}\right)\mathbf{b}_n=0. \tag{8a}$$

Alternatively, we could have transformed the relation (2a) using the transformation (6b). We would then have found

$$\left(A_{ri}A_{mj}\epsilon_{rmn}-\frac{p}{p'}\epsilon_{ijk}A_{nk}\right)\mathbf{b}'_n=0. \tag{8b}$$

In eqs (8) we have vanishing linear combinations of each set of basis vectors. Since the vectors in each set are linearly independent, the coefficients in each linear combination must vanish identically. This leads to

$$A_{ir}A_{jm}\epsilon_{rmn}=\frac{p'}{p}\epsilon_{ijk}A_{kn}, \tag{9a}$$

$$A_{ri}A_{mj}\epsilon_{rmn}=\frac{p}{p'}\epsilon_{ijk}A_{nk}. \tag{9b}$$

These equations, which we shall refer to as the second orthogonality conditions, appear to be new, or at any rate do not appear to have been discussed before. In the next section we will work out their main consequences.

3. Consequences of the Second Orthogonality Conditions

As a first consequence of eqs (9), we construct a vector which is not altered by the transformation represented by A. To do this, we contract on i and n in eq (9a), that is, we set $i=n$ and sum on the repeated index so formed. Now the Levi-Civita symbol has the same value for any cyclic permutation of its indices. For example

$$\epsilon_{njk}=\epsilon_{jkn}. \tag{10}$$

Therefore we may write the contracted form of eq (9a) as

$$A_{jm}(\epsilon_{mnr}A_{nr})=\frac{p'}{p}\epsilon_{jkn}A_{kn}. \tag{11}$$

By defining the three component quantity $\mathbf{V}_m$ as

$$\mathbf{V}_m \equiv \epsilon_{mnr} A_{nr}, \tag{12}$$

we may write eq (11) in the form

$$A_{jm}\mathbf{V}_m = \frac{p'}{p}\mathbf{V}_j. \tag{13a}$$

This equation says that unless it is identically zero, the "vector" $\mathbf{V}$ is an eigenvector of A belonging to the eigenvalue p'/p. Similarly, contracting on i and n in eq (9b), and observing that $p/p' = p'/p$, we find

$$A_{mj}\mathbf{V}_m = (\tilde{A})_{jm}\mathbf{V}_m = \frac{p'}{p}\mathbf{V}_j. \tag{13b}$$

so that $\mathbf{V}$ is also an eigenvector of the matrix $\tilde{A}$, the transpose of A, belonging to the same eigenvalue p'/p.

Of course $\mathbf{V}$ is not the only real eigenvector of A and of $\tilde{A}$ belonging to the eigenvalue p'/p. Because of the homogeneity of eqs (13) any non-null vector parallel or antiparallel to $\mathbf{V}$ is an eigenvector. For example if $\mathbf{V}$ is not identically zero, a unit vector may be formed from it by dividing $\mathbf{V}$ by its length. In the case of rigid rotations, for which $p'/p = 1$, this unit vector specifies the direction of the axis of rotation, and the development embodied in eqs (11) through (13) can be taken as a new proof of Euler's theorem [5]. The significance of the particular vector $\mathbf{V}$ for rigid rotations is that is gives not only the axis of rotation but the sine of the angle of rotation as well. When combined with the cosine of the angle of rotation as derived from the trace of A, this gives directly the complete, unambiguous correlation between the axis and angle of rotation. This will be seen in the second paper in this series, where eqs (13) and the vector $\mathbf{V}$ are considered in detail. In particular, it will be shown that $\mathbf{V}$ can be expressed as

$$\mathbf{V} = 2\mathbf{n} \sin \alpha,$$

where $\mathbf{n}$ is a unit vector giving the direction and the chosen sense of the axis of rotation, and α is the angle of rotation whose sense of description about the axis agrees with the handedness of the coordinate system which is rotated by A.

Although the derivations of eqs (12) and (13) from the second orthogonality relations are new, most of the results of those equations are not new. In particular, the fact that the ratios of the components of any vector which specifies the axis of a rigid rotation are identical to the ratios of the components of $\mathbf{V}$, has been known for a long time [6, 7]. This result has unfortunately not been adequately stressed in the literature. We would like to call attention to it here and to emphasize the slightly more general conclusion that eqs (12) and (13) form a prescription for writing down real eigenvectors of a transformation matrix without in fact solving the eigenvalue equation for the matrix. The prescription fails of course when $\mathbf{V}$ vanishes identically. As can be seen from eq (12), this occurs whenever A is symmetric in addition to being orthogonal. In paper II we shall see that a symmetric A corresponds to a rigid rotation of either 0° or 180° for the proper rotations ($p'/p = 1$), and to either a reflection in a plane or to an inversion of the coordinate system with respect to the origin, for the improper rotations ($p'/p = -1$). In such instances one must solve the eigenvalue equation for A to find its real eigenvectors.

We have been referring to $\mathbf{V}$ as a vector since it is a three-component object. However, it is not a vector in the sense in which the physicist usually understands that word. He would think of a vector as a one-to-one correspondence between coordinate systems and sets of three numbers,

which under a transformation of coordinates obeys the transformation law of coordinate intervals.[3] Strictly speaking, **V** has relevance to the transformation between two coordinate systems, rather than as an object germane to individual coordinate systems. For convenience, however, we will continue to refer to **V** as a vector, keeping in mind its limitations under the transformation definition. For want of a better name, we shall henceforth call **V** the intrinsic vector.

The second consequence of eqs (9) that we shall derive is a new equation which connects the trace of A, tr A, with tr (A^2). To find it, we multiply eq (9a) by ϵ_{ijn}, and sum on i, j, and n. With the aid of the identities [4]

$$\epsilon_{ijn}\epsilon_{rmn} = \delta_{ir}\delta_{jm} - \delta_{im}\delta_{jr}, \tag{14a}$$

$$\epsilon_{ijn}\epsilon_{ijk} = 2\delta_{nk}, \tag{14b}$$

we arrive at

$$A_{ii}A_{jj} - A_{ij}A_{ji} = 2\frac{p'}{p}A_{nn}.$$

In trace notation this equation appears as

$$(\mathrm{tr}\,A)^2 - \mathrm{tr}\,(A^2) = 2\frac{p'}{p}\mathrm{tr}\,A. \tag{15}$$

Equation (15) can also be derived by similar operations on eq (9b).

The trace of a transformation matrix is primarily important for rigid rotations, where it furnishes the cosine of the angle α of rotation by means of the well known formula

$$\mathrm{tr}\,A = 1 + 2\cos\alpha. \tag{16}$$

The standard derivation of this formula [5] makes use of the special form of a rotation matrix when the axis of rotation is one of the coordinate axes, say the z axis. By direct calculation of the underlying two-dimensional transformation, this matrix is seen to be

$$\begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv R_z(\alpha). \tag{17}$$

The trace of this matrix is given by eq (16). It is then noted that *any* rotation matrix may be put into the form (17) by an appropriate similarity transformation. The result (16) for an arbitrary rotation matrix then follows from the fact that the trace of a matrix is invariant under a similarity transformation.[5]

---

[3] I am indebted to Robert Richtmeyer, from whom I first heard this particular wording of the transformation definition of a vector.

[4] An elementary and very lucid introduction to the use of the Levi-Civita symbol can be found in ref. [8]. This includes a derivation of the identity (14a), from which the identity (14b) may be derived by further contraction.

[5] In the language of group theory, real three-by-three orthogonal matrices belong to the vector representation, or the irreducible representation corresponding to $l = 1$, of the rotation group. The characters of a representation are the traces of its matrices. Equation (16) is true only for the characters of the vector representation. For the matrices of the irreducible representation belonging to integral $l \geq 1$ the characters are given by $1 + 2\cos\alpha + \ldots + 2\cos l\alpha$, where α is the angle of rotation.

It is possible to derive the formula for the trace analytically from eq (15) using only general properties of rotations, and without the need to consider special forms of the rotation matrix. The derivation is interesting because it shows that the formula (16) is a direct consequence of the algebraic properties of rotation matrices, and so gives an insight into the structure of that formula which one does not get from the standard derivation. The details of the derivation of eq (16) from eq (15) will be presented in paper IV.

As a third consequence of eqs (9) we deduce a transparent expression for the determinant of A, det A. We first note that the properties of determinants furnish the identities [6]

$$A_{ir}A_{jm}A_{sn}\epsilon_{rmn} = (\det A)\,\epsilon_{ijs}, \tag{18a}$$

$$A_{ri}A_{mj}A_{ns}\epsilon_{rmn} = (\det A)\,\epsilon_{ijs}. \tag{18b}$$

If we then multiply either eq (9a) by A_{sn} or eq (9b) by A_{ns} and sum on s then the left side of either of the resulting equations is, by eqs (18), equal to (det A) ϵ_{ijs}. The right sides each lead to (p'/p) ϵ_{ijs}, with the help of the first orthogonality conditions (7). Equating these two expressions we have

$$\det A = \frac{p'}{p}. \tag{19}$$

This equation states in a concise form the result that the determinant of a real three-by-three orthogonal transformation matrix is equal to $+1$ when the transformation does not cause a change in handedness, and equal to -1 when it does. This result is of course well known but does not emerge quite as concisely in the customary way of deriving it. There, one uses the first orthogonality conditions to arrive at the result $(\det A)^2 = 1$, from which it follows that $\det A = \pm 1$. One then argues that only for the proper rotations is A continuously connected to the identity matrix, for which the determinant is $+1$. This leaves the value -1 of the determinant to account for the improper rotations. The second orthogonality conditions lead to these conclusions in a single succinct equation.

The final result of this section is a derivation of the secular equation for a transformation matrix, directly from the second orthogonality conditions. A word of clarification is in order. By the phrase "secular equation" of a matrix, one usually means the polynomial equation obeyed by the eigenvalues of the matrix. The Cayley-Hamilton theorem [10] asserts that the matrix itself obeys its own polynomial equation. For this reason we refer to the polynomial equation satisfied by a transformation matrix as its secular equation. It is in this form that the secular equation for A comes out of eqs (9).

We multiply eq (9a) by ϵ_{stn}, and sum on n using the identity (14a). This gives

$$A_{is}A_{jt} - A_{it}A_{js} = \frac{p'}{p}\,\epsilon_{ijk}\epsilon_{stn}A_{kn}. \tag{20}$$

We now contract this equation on s and j. To evaluate the right side of the contracted equation we use the cyclic property (10) of ϵ and the identity (14a). The result is

$$(A^2)_{it} - (\mathrm{tr}\,A)A_{it} = \frac{p'}{p}\,[A_{ti} - (\mathrm{tr}\,A)\delta_{it}].$$

The matrix form of this equation is

$$A^2 - (\mathrm{tr}\,A)A = \frac{p'}{p}\,[\tilde{A} - (\mathrm{tr}\,A)I], \tag{21}$$

[6] A derivation of these identities may be found in ref. [9]. In the theory of Cartesian tensors, these identities constitute the proof that the Levi-Civita symbol is a pseudotensor of the third rank.

where $\tilde{A}$ is the transpose of A, and I is the identity matrix. Upon multiplying eq (21) by A, either from the left or from the right, and noting that $A\tilde{A}=\tilde{A}A=I$ from the first orthogonality relations, we have

$$A^3-(\mathrm{tr}\,A)A^2+\frac{p'}{p}(\mathrm{tr}\,A)A-\frac{p'}{p}I=0. \tag{22}$$

This is the secular equation for A.

For the special case of rigid rotations, we can set $p'/p=1$, and use eq (16) for tr A, in eq (22). The secular equation for a rotation matrix is then

$$A^3-(1+2\cos\alpha)A^2+(1+2\cos\alpha)A-I=0. \tag{23}$$

This may be written in the factored form

$$(A-I)[A^2-(2\cos\alpha)A+I]=0. \tag{24}$$

If A in eq (23) (or eq (24)) is replaced by a numerical variable representing the eigenvalues of A, then the solution of the resulting equation gives the usual result that the eigenvalues are 1, $e^{i\alpha}$, and $e^{-i\alpha}$. The fact that one of the eigenvalues is unity may be taken as yet another direct proof from eqs (9) of Euler's theorem. This proof has the advantage over the one based on eqs (13) in that it remains valid even when the intrinsic vector vanishes.

A more powerful use of eq (23) is in finding a closed-form expression for A as a function of the axis and angle of rotation. On the basis of very general properties of rotation matrices, the solution of eq (23) is

$$A(\alpha)=I-N\sin\alpha+N^2(1-\cos\alpha). \tag{25}$$

Here, N is a matrix which is formed from the components of **n**, the unit vector along the sense of the axis of rotation, by the prescription

$$N_{ik}\equiv\epsilon_{ijk}n_j. \tag{26}$$

In explicit matrix form, N appears as

$$N=\begin{pmatrix}0 & -n_3 & n_2\\ n_3 & 0 & -n_1\\ -n_2 & n_1 & 0\end{pmatrix}. \tag{27}$$

Equation (25) is probably more familiar in its exponential form.[7]

$$A(\alpha)=e^{-N\alpha}. \tag{28}$$

Since eq (23) is independent of the axis of rotation, it is to be expected that it has to be supplemented by a condition which introduces the axis. The appropriate condition is the eigenvalue equation for A corresponding to the eigenvalue $+1$.

The details of how eq (23) is solved to give eq (25) are interesting in their own right, and are given in paper IV. As with the solution of eq (15) to yield the trace formula, the process of solving

[7] The reader who is familiar with the dyadic representation of rotations will recognize the similarity between eq (25) and the rotation dyadic [11]. The matrix N is replaced by the dyadic $-\mathbf{n}\times\mathbf{I}$, where $\mathbf{I}$ is the unit dyadic, the minus sign entering because a dyadic is generally used to describe an active transformation, whereas eq (25) is meant to describe a passive transformation. The matrix N^2 is replaced by the dyadic $\mathbf{n}\times(\mathbf{n}\times\mathbf{I})$ which is just $(-\mathbf{n}\times\mathbf{I})\cdot(-\mathbf{n}\times\mathbf{I})=(-\mathbf{n}\times\mathbf{I})^2$. One can check that the matrix form of $\mathbf{n}\times\mathbf{I}$ is given by the right side of eq (26).

eq (23) from general properties of rotations shows the intimate connection between the result, eq (25), and the algebraic properties of rotation matrices. As will be seen in paper IV, the same general properties of rotations are invoked to solve both eqs (15) and (23). These are the group property, and the periodicity property.

In all of the results derived in this section, it can be seen that the only way in which p and p' occur is in the ratio p'/p. This is an expression of the fact that only the relative handedness of two coordinate systems is of any significance. To emphasize this fact we shall continue to write the ratio as p'/p, rather than define a new symbol for it.

We have already indicated the contents of papers II and IV of this series. Paper III will be concerned with the proof of the theorem of conjugacy, from the second orthogonality conditions. This theorem makes statements about the axes and angles of rotation of two rotation matrices connected by an orthogonal similarity transformation.

I would like to thank Monte A. Franklin, Kent R. Johnson, Nicholas M. Tomljanovich, and Peter C. Waterman for critically reading an earlier version of this paper, and for making a number of useful suggestions. I am grateful to Werner E. Sievers and William A. Whitcraft, Jr. for their encouragement during the course of this work.

4. References

[1] Page, L., Introduction to Theoretical Physics, 3rd ed., sec. 18 (D. Van Nostrand Company, Inc., New York, 1952).
[2] Corben, H. C., and Stehle, P., Classical Mechanics, 2nd ed., appendix IV (John Wiley and Sons, Inc., New York, 1960).
[3] Carruthers, P., Introduction to Unitary Symmetry, sec. 1.1 (Interscience Publishers, New York, 1966).
[4] Goldstein, H., Classical Mechanics, chap. 4 (Addison-Wesley Publishing Company, Reading, Massachusetts, 1953).
[5] Goldstein, H., op. cit., sec. 4–6.
[6] Wigner, E. P., Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra, sec. 14–7 (Academic Press, New York, 1959).
[7] Hamermesh, M., Group Theory, sec. 9–2 (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1962).
[8] Evett, Arthur A., Permutation symbol approach to elementary vector analysis, Am. J. Phys. **34**, 503 (1966).
[9] Goertzel, G., and Tralli, N., Some Mathematical Methods of Physics, appendix 1A (McGraw-Hill Book Company, Inc., New York, 1960).
[10] Hoffman, K., and Kunze, R., Linear Algebra, sec. 6.2 (Prentice-Hall Publishing Company, Inc., Englewood Cliffs, New Jersey, 1961).
[11] Page, L., op. cit., sec. 18.2.

(Paper 72B3–272)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 3, July–September 1968

Thickness and Connectivity in Graphs

Arthur M. Hobbs and J. W. Grossman

Institute for Applied Technology, National Bureau of Standards, Washington, D.C. 20234

(June 25, 1968)

A graph G has *thickness* t if and only if t is the smallest number of planar subgraphs of G whose union is G. A *thickness-minimal*, or *t-minimal*, graph is a graph of thickness t with no proper subgraph of thickness t. In this paper we show that, for every t, a cut set in a t-minimal graph can have no fewer than t edges. This theorem suggests that the connectivity of a t-minimal graph is bounded from below by t. We disprove this suggestion for every $t > 2$ by constructing a graph which contains a 2-connected t-minimal graph. Two theorems extend this result and develop additional properties of the construction method. In addition, we show that the connectivity of a graph of thickness t is at most $6t-1$ and that the thickness of K_{22} is 4. Finally, we make four conjectures about graphs of thickness t.

Key Words: Conjectures, connectivity, cut-set, graph theory, mathematics, minimality, thickness of graphs.

1. Definitions and Previous Results

A *graph* is a finite set of points, called *vertices*, together with a finite set of line segments, called *edges*, such that each end point of an edge is a vertex, no edge meets more than two vertices, and edges meet only at end points. If two edges share an end point, they are *adjacent*. The end points of an edge are said to be *joined* by the edge. A *subgraph* of a graph G is a subset of the edges and vertices of G which is again a graph.

A graph is *complete* if and only if every pair of vertices is joined by an edge; a complete graph with n vertices is denoted by K_n. A graph G is *bipartite* if and only if there is a separation of the vertices of G into two disjoint sets A and B such that every edge of G joins a vertex in A with a vertex in B. A bipartite graph is *complete* if and only if every vertex in A is joined to every vertex in B by an edge; such a graph is denoted by $K_{m,n}$, where m is the number of vertices in the set A and n is the number of vertices in the set B.

A graph is *planar* if and only if it can be drawn in the plane in such a way that no two distinct points of the graph occupy the same point of the plane. The *union* of subgraphs $H_1, H_2, \ldots, H_n$ of a graph G is the subgraph of G consisting of all edges and all vertices from the H_i. The *thickness* $\theta(G)$ of a graph G is defined [5] as the minimum number of planar subgraphs whose union is G. A *thickness-minimal*, or *t-minimal*, graph is a graph of thickness t which contains no proper subgraph of thickness t.

A (simple) *path* in G is a vertex, a single edge, two adjacent edges, or a subset $e_1, e_2, \ldots, e_n$, $n > 2$, of the edges of G such that e_{i+1} joins an end point of e_i with an end point of e_{i+2}, $i = 1, 2, \ldots, n-2$, and no vertex is the end point of more than two edges of the path. The path is said to *join* any two vertices met by edges of the path. A *circuit* is a path such that e_1 and e_n are adjacent. A graph or subgraph G is *connected* if and only if for any two vertices of G there exists a path in G joining the two vertices. The *girth* of a graph G is the smallest integer n such that there exists a circuit in G having n edges.

312-532 O - 68 - 6

A *component* of a graph G is a maximal connected subgraph of G. The *connectivity* of a connected graph G is the smallest number of vertices of G whose removal (together with all edges meeting at least one of the vertices) leaves a subgraph of G which has no edges or which is not connected. If G is not connected, it has connectivity 0. An *articulation point* of a graph G is a vertex whose removal from G (together with all incident edges) increases the number of components in the remaining graph. A *cut set* of a graph G is a subset S of the edges of G whose removal disconnects G and such that no proper subset of S has the same property.

W. T. Tutte [5][1] proved several theorems which we have found very useful. We state those theorems here with their original numbering:

(3.1) Let G be a graph of thickness t. Let G' be formed from G by deleting either a single edge or a single vertex with all its incident edges. Then the thickness of G' is either t or $t-1$. (In particular, if G is t-minimal, then $\theta(G')=t-1$.)

(3.2) Let k be a nonnegative integer and let G be a graph of thickness $t \geq k$. Then there exists a k-minimal subgraph of G.

(3.3) Every t-minimal graph is connected and nonseparable. (A graph is nonseparable if and only if it is connected and contains no articulation points.)

(5.3) For each integer $t \geq 2$ there exist infinitely many nonisomorphic t-minimal graphs of upper valency $2t-1$, and of girth greater than any specified integer N.

2. Connectivity and Thickness

The *valency* of a vertex of a graph G is the number of edges incident on the vertex. Let v be the least integer occurring as the valency of a vertex of G. W. T. Tutte has shown [5] that if G is a t-minimal graph, $t>0$, then $v \geq t$. The following generalizes Tutte's result:

THEOREM 1: *Let* G *be* t*-minimal*, t >0, *and let* n *be the number of edges in a cut set of* G. *Then* n $\geq$ t.

PROOF: Suppose G has a cut set S with $k<t$ edges in it. Let the vertices of G be partitioned into the sets A and B by S. Obtain G' by removing one edge $e=(a, b) \epsilon S$ from G. Since G is t-minimal, $\theta(G')=t-1$, and we can find $t-1$ planar subgraphs $H_1, H_2, \ldots, H_{t-1}$ of G' whose union is G'. We may assume that no edge of G' appears in more than one of the H_i. There are only $k-1<t-1$ edges of S in G', so one of the H_i, say H_1, must not contain any edge of S. Because S is a cut set of G, H_1 (which we may assume contains all the vertices of G) must be disconnected with vertex a in one component and vertex b in some other component. Using stereographic projection, we may draw the component containing vertex a in the plane so that a is on the boundary of the infinite region of the component, and similarly with the component containing vertex b. Then a new planar subgraph H_1' can be formed from H_1 by joining vertices a and b by edge e. But the union of H_1' together with $H_2, \ldots, H_{t-1}$ is G, thus giving a partition of G into $t-1$ planar subgraphs, contrary to hypothesis. Q.E.D.

Given the result of Theorem 1, we might conjecture that the connectivity of a t-minimal graph is bounded from below by t. However, for all $t>2$, the following propositions show this conjecture to be false.

Let us define an operation on two disjoint graphs G_1 and G_2 as follows: choose an edge $e_i=(a_i, b_i)$ from graph G_i, delete edge e_i from G_i, and identify a_1 with a_2 and b_1 with b_2, obtaining a graph $J(G_1, G_2)$ called the *join* of G_1 and G_2. Note that if G_1 and G_2 each have connectivity at least 2, then $J(G_1, G_2)$ has connectivity exactly 2. In general there are many different joins of two graphs, depending on the choice of edges e_1 and e_2. However, in this paper we are concerned only with those properties of the join which are independent of the choice of the two edges. Let us denote the vertex resulting from identifying a_1 and a_2 by a, and that from b_1 and b_2 by b. The subgraph of $J(G_1, G_2)$ corresponding to $G_1-\{e_1\}$ we denote by G_1' and that corresponding to $G_2-\{e_2\}$ by G_2'. Since the thickness of a graph is reduced at most 1 by the removal of an edge, it is clear that $\theta(J(G_1, G_2)) \geq \max(\theta(G_1), \theta(G_2))-1$.

[1] Figures in brackets indicate the literature references at the end of this paper.

LEMMA: *If* $\theta(G_1)=\theta(G_2)=t$, *then any join of* G_1 *and* G_2 *has thickness* t *or* $t+1$.

PROOF: Remove vertices a and b and all incident edges from $J(G_1, G_2)$. In the resulting graph every component is a proper subgraph of G_1' or G_2' and can therefore be partitioned into t or fewer planar subgraphs. Since $K_{2,m}$ is planar for every integer m, we can place a and b with their incident edges in one additional plane. Thus, $\theta(J(G_1, G_2)) \leq t+1$.

But suppose $J(G_1, G_2)$ can be partitioned into $t-1$ planar subgraphs $H_1, \ldots, H_{t-1}$. The subgraph G_i' of $J(G_1, G_2)$ together with the additional edge (a, b) is isomorphic to G_i for each i. Since G_i has thickness t, $H_1 \cap G_1'$ together with edge (a, b) cannot be planar. Hence in any embedding of $H_1 \cap G_1'$ in the plane there is a circuit C composed entirely of edges and vertices of $H_1 \cap G_1'$ such that a and b are in different components of the plane if C is removed from it.

Supposing that a and b are not joined by a path in $H_1 \cap G_2'$ they must be in separate components thereof. We can then draw each in the plane in such a way as to place a and b on the boundaries of their components and join them by an edge. Thus we obtain a partition of G_2 into $t-1$ planar subgraphs. Therefore, a path P having more than one edge joins a with b and lies entirely within $H_1 \cap G_2'$. Now P must cross C in H_1. By the Jordan curve theorem, P and C must share a point, and by the definition of planar embedding of graphs, that point must be a vertex of G other than a and b. But a and b are the only vertices shared by G_1' and G_2'. Hence, $\theta(J(G_1, G_2)) \geq t$. Q.E.D.

THEOREM 2: *For every* $t \geq 2$, *there exists a* t*-minimal graph with connectivity 2.*

PROOF: If G_i is t-minimal, G_i' cannot include a t-minimal subgraph. But since $\theta(J(G_1, G_2)) \geq t$, there exists a t-minimal subgraph K contained in $J(G_1, G_2)$ (Theorem 3.2 of [5]). Clearly this t-minimal subgraph includes one or both of a and b, as well as other vertices from each of the G_i'. But Theorem 3.3 of [5] states that K cannot have an articulation point. Therefore, both a and b are contained in K, and K has connectivity 2. Q.E.D.

The results of Tutte's paper [5] allow us to extend the above theorem much farther. Denote the girth of G_i by $g(G_i)$.

THEOREM 3: *For each integer* $t \geq 2$ *and* $N \geq 2$, *there exists a* t*-minimal graph of connectivity 2 with girth greater than* N.

PROOF: $J(G_1, G_2)$ cannot have girth less than min $(g(G_1), g(G_2))$, since the only circuits of G_i affected by the join are those including edge (a_i, b_i), and those circuits are increased by at least one edge in the join. Thus, for all graphs G_1 and G_2, $g(J(G_1, G_2)) \geq \min(g(G_1), g(G_2))$. By Theorem 5.3 of [5], given an integer N, there exists a t-minimal graph G with girth greater than N. Then $g(J(G, G)) \geq g(G) > N$. Since any subgraph of a graph of girth m has girth at least m, for any t-minimal subgraph K contained in $J(G, G)$, $g(K) > N$, and, by Theorem 2, the connectivity of K is 2. Q.E.D.

COROLLARY: *For every* $t \geq 2$ *there exists an infinite class of nonisomorphic* t*-minimal graphs, each having connectivity 2.*

THEOREM 4: *Let* G_1 *be* t*-minimal and* $\theta(G_2)=t$. *Then* $\theta(J(G_1, G_2))=t$.

PROOF: Partition G_2 into t planar subgraphs H_i such that a_2 and b_2 are on the boundary of the same region in one of the subgraphs, say H_1 (this is possible since G_2 has thickness t with edge (a_2, b_2) present). Remove vertices a_1 and b_1 and all incident edges from G_1. Since G_1 is t-minimal, the resulting graph G_1'' has thickness $t-1$ or less. Partition G_1'' into $t-1$ planar subgraphs and assign one of these subgraphs to each of the $t-1$ planar subgraphs of G_2 other than H_1. Now it is trivial to embed $K_{2,n}$ in the plane so that the two vertices in the first subset are on the boundary of the infinite region. Hence we may identify a_1 with a_2 and b_1 with b_2 in subgraph H_1 of G_2, placing all edges joined to either a_1 or b_1 in that subgraph. The result is an embedding of $J(G_1, G_2)$ (together with edge (a, b)!) in t planes, and by Theorem 2, $\theta(J(G_1, G_2))=t$. Q.E.D.

Having answered the question of the lower bound for the connectivity of a t-minimal graph, it is natural for us to ask for an upper bound for the connectivity of a graph of thickness t. Such an upper bound can be easily derived by the use of Euler's formula for planar graphs as follows. Let $E(G)$ be the set of edges of a graph G and $V(G)$ the set of vertices of G. Denote the number of elements of a set S by $|S|$.

THEOREM 5: *Let* $\theta(G)=t>0$. *Then there is a vertex of valency less than or equal to* $6t-1$ *in* G.

PROOF: Suppose the smallest valency in G is m. Then

$$|E(G)| \geq \tfrac{1}{2} m|V(G)|. \tag{1}$$

Since $\theta(G)=t$, there exist t planar subgraphs $H_1, \ldots, H_t$ of G whose union is G. By Euler's formula in each planar subgraph,

$$|E(H_i)| \leq 3|V(H_i)|-6=3|V(G)|-6,$$

since we may assume that every H_i contains all of the vertices of G. Thus,

$$|E(G)| \leq 3t|V(G)|-6t. \tag{2}$$

Combining (1) and (2),

$$\tfrac{1}{2} m|V(G)| \leq 3t|V(G)|-6t.$$

Rearranging terms,

$$|V(G)|(\tfrac{1}{2} m-3t) \leq -6t.$$

Since $|V(G)|$ and t are both positive for $t>0$,

$$\tfrac{1}{2}m-3t<0,$$

or

$$m \leq 6t-1. \qquad \text{Q.E.D.}$$

COROLLARY: *The connectivity of a graph of thickness* t *is less than or equal to* $6t-1$.

3. Conjectures

1. There are no G_1 and G_2 with $\theta(G_1)=\theta(G_2)=t$ such that $\theta(J(G_1, G_2))=t+1$. This conjecture is certainly true for $t=1$. For $t>1$, we have been unable to find a counterexample.

2. We have shown in a previous paper [3] that $K_{4t-5,\,4t-5}$ is t-minimal for all $t \geq 2$. By taking $J(K_{4t-5,\,4t-5}, K_{4t-5,\,4t-5})$ and finding a t-minimal subgraph, we obtain a t-minimal bipartite graph which is not a complete bipartite graph. It would be interesting for each t to characterize the class of all t-minimal bipartite graphs.

The 2-minimal bipartite graphs are easily characterized. Kuratowski [4] proved that every 2-minimal graph is homeomorphic to K_5 or $K_{3,3}$. If G is bipartite, let the vertices of G be partitioned into sets A and B such that all edges of G join a vertex in A with one in B. Clearly any path joining a vertex in A with a vertex in B contains an odd number of edges (= even number of vertices), while a path joining a vertex in one of the sets A or B with another vertex in the same set contains an even number of edges (= odd number of vertices). To generate all 2-minimal bipartite graphs, start with one of K_5 or $K_{3,3}$ and write down a partition of its vertices into two sets. With respect to the given partition, an edge joining two vertices in the same set may be replaced by a path consisting of valence 2 vertices and an even number of edges without destroying 2-minimality. Likewise edges joining vertices in different sets may be replaced by paths consisting of valence 2 vertices and an odd number of edges, or by a single edge. The set of all graphs generated by all such replacements in all such partitionings of both K_5 and $K_{3,3}$ constitutes the complete set of 2-minimal bipartite graphs.

3. Let $N(t)$ be the smallest integer such that there exists a t-minimal graph having $N(t)$ vertices. We know that $N(2)=5$ (reference [4]) and $N(3)=9$ (reference [6]). Beineke and Harary [1] have shown that $6t-8 \leq N(t) \leq 6t-7$ for all $t \geq 4$. Since $\theta(K_{22})=4$ (see appendix A), $N(5)=6(5)-7=23$. Beineke has shown [8] that $\theta(K_{28})=5$, from which it follows that $N(6)=29$. In accordance with Harary's conjecture [7] that $\theta(K_{16})=4$, we conjecture that $N(4)=16$ and $N(t)=6t-7$ for all $t \geq 5$.

4. For all $n \geq N(t)$, there exists a t-minimal graph having exactly n vertices.

This conjecture is certainly true for $t=2$. For $t>2$, an immediate consequence of Theorem 5.3 of [5] is that for every $n \geq N(t)$, there exists a t-minimal graph having at least n vertices. Further evidence about the conjecture is lacking, and it does not appear to be easily proven if true. Unfortunately, because of the difficulty in establishing the thickness and t-minimality of most graphs, the conjecture is not likely to be easily disproven either.

4. Appendix A

In their paper on the thickness of the complete graph [1], Beineke and Harary were unable to give the thickness of the graphs K_n for $n \geq 16$ with $n \equiv 4 \pmod 6$, except for the case of K_{28}

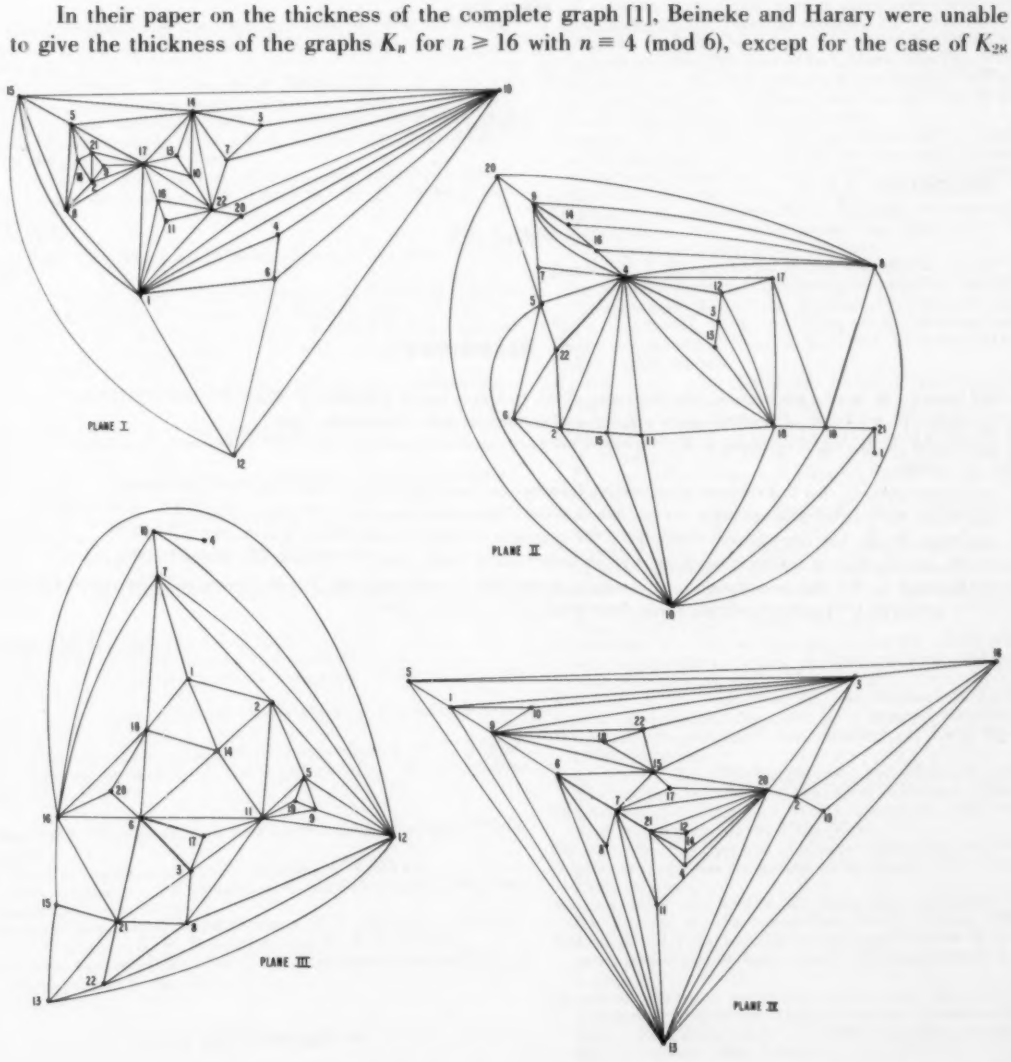

FIGURE 1. K_{22} *in four planes.*

whose thickness they found by trial and error to be 5. To provide additional data for those who are attempting to determine the thickness of this class of complete graphs, we include the following:

THEOREM: $\theta(K_{22})=4$.

PROOF: Figure 1 shows four planar graphs whose union is K_{22}. By Euler's formula,

$$|E(K_{22})| \leq 3t|V(K_{22})| - 6t = 60t.$$

But

$$|E(K_{22})| = 231.$$

Thus,

$$60t \geq 231,$$

or

$$t \geq 4.$$

Therefore,

$$\theta(K_{22}) = 4. \qquad \text{Q.E.D.}$$

5. References

[1] Beineke, L. W., and F. Harary, The thickness of the complete graph, Canadian J. Math. **17**, 850–859 (1965).

[2] Dirac, G. A., Short proof of Menger's graph theorem, Mathematika **13**, 42–44 (1966).

[3] Hobbs, A. M., and Grossman, J. W., A class of thickness-minimal graphs, J. Res. NBS **72B** (Math. Sci.) No. 2, 145–153 (1968).

[4] Kuratowski, C., Sur le Problème des Courbes Gauches en Topologie, Fund. Math. **15**, 271–283 (1930).

[5] Tutte, W. T., The thickness of a graph, Nederl. Akad. Wetensch. Proc. Ser. A66 Indag. Math. **25**, 567–577 (1963).

[6] Tutte, W. T., The non-biplanar character of the complete 9-graph, Canad. Math. Bull. **6**, 319–330 (1963).

[7] Harary, F., Recent results in topological graph theory, Acta Math. Acad. Sci. Hung. **15**, 405–412 (1964).

[8] Beineke, L. W., The decomposition of complete graphs into planar subgraphs, Graph Theory and Theoretical Physics, edited by F. Harary, Academic Press, New York, N.Y., 139–153 (1967).

(Paper 72B3–273)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 3, July–September 1968

Publications of the National Bureau of Standards*

J. Res. NBS 72A (Phys. and Chem.), No. 3, (May–June 1968), $1.00

Jump rates for point defects in special positions held by a trapping center of noncubic symmetry. H. S. Peiser and J. B. Wachtman Jr.

The thermodynamics of the ternary system: water-potassiun chloride-calcium chloride at 25 °C. R. A. Robinson and A. K. Covington.

Force field for SiF_4. I. W. Levin and S. Abramowitz.

Blemish formation in processed microfilm. C. I. Pope.

Absolute isotopic abundance ratios of common, equal-atom, and radiogenic lead isotopic standards. E. J. Catanzaro, T. J. Murphy, W. R. Shields, and E. L. Garner.

Role of nickel in Al-10 percent Si composites containing nickel-coated sapphire whiskers. H. Yakowitz, W. D. Jenkins, and H. Hahn.

J. Res. NBS 72A (Phys. and Chem.), No. 4, (July–Aug. 1968), $1.00

Mass spectrometric study of photoionization. X. Hydrogen chloride and methyl halides. M. Krauss, J. A. Walker, and V. H. Dibeler.

The fourth and fifth spectra of vanadium (V IV and V V). L. Iglesias.

Variation of absorptance-curve shape with changes in pigment concentration. G. L. Howett.

Periodic acid, a novel oxidant of polycyclic aromatic hydrocarbons. A. J. Fatiadi.

A galvanic cell with a low emf-temperature coefficient. G. N. Roberts and W. J. Hamer.

Synthesis of cerite. J. Ito.

Tables of collision integrals of the $(m, 6)$ potential function for values of m. M. Klein and F. Smith.

Spectrum of relaxation times in GeO_2 glass. A. Napolitano and P. B. Macedo.

Resumé of values of the Faraday. W. J. Hamer.

J. Res. NBS 72C (Engr. and Instr.), No. 2, (Apr.–June 1968), 75 cents.

Analysis and design of an oscilloscope deflection system with a calculable transfer function. D. M. Stonebraker.

Calculation of substitution error in barretters. S. Jarvis, Jr., and J. W. Adams.

Analysis of n-degree elliptical elastic rings of nonuniform cross section. R. A. Mitchell.

Applications of coaxial chokes to a-c bridge circuits. D. N. Homan.

Creep rupture properties of Ti-8Al-1Mo-IV alloy. W. D. Jenkins and W. A. Willard.

J. Res. NBS 72C (Engr. and Instr.), No. 3, (July–Sept. 1968), 75 cents.

Gas density balance design considerations. E. C. Creitz.

Standard mismatch—the production of controlled small reflections in waveguides. L. Lewin.

Viscoelastic behavior of dental amalgam. P. L. Oglesby, G. Dickson, M. L. Rodriguez, R. M. Davenport, and W. T. Sweeney.

The steady-state creep behavior of dental amalgam. George Dickson, P. Oglesby, and R. Davenport.

Other NBS Publications

Brennan, J. A., Edmonds, D. K., and Smith, R. V., Two-phase (liquid-vapor), mass-limiting flow with hydrogen and nitrogen, Tech. Note 359 (Jan. 30, 1968), 25 cents.

Blaine, R. L., Arni, H., and DeFore, M. R., Interrelations between cement and concrete properties. Part 3, compressive strengths of portland cement test mortars and steam-cured mortars, Bldg. Sci. Series 8 (Apr. 1968), 55 cents.

Corliss, C. H., and Tech. J. L., Oscillator strengths and transition probabilities for 3288 lines of Fe I, Mono. 108 (Mar. 1968), 45 cents.

Freeman, D. H., Ed., Separation and Purification Section: Summary and initial activities February 1966 through June 1967, Tech. Note 429 (Feb. 1968), 35 cents.

Furukawa, G. T., Saba, W. G., and Reilly, M. L., Critical analysis of the heat-capacity data of the literature and evaluation of thermodynamic properties of copper, silver, and gold from 0 to 300 °K, Natl. Std. Ref. Data Series 18 (Apr. 1968), 40 cents.

Glennon, B. M., and Wiese, W. L., Bibliography on atomic transition probabilities, May 1966 through December 1967, Misc. Publ. 278 Supplement (Apr. 1968), 30 cents.

Hanley, H. J. M., and Klein, M., On the selection of the intermolecular potential function: Application of statistical mechanical theory to experiment, Tech. Note 360 (Nov. 20, 1967), 50 cents.

Ho, C. Y., Powell, R. W., and Liley, P. E., Thermal conductivity of selected materials, Part 2, Natl. Std. Reference Data Series 16 (Feb. 1968), $2.00.

Kneissl, G. J., and Richmond, J. C., A laser-source integrating sphere reflectometer, Tech. Note 439 (Feb. 1968), 45 cents.

Lee, R. W., and Worral, R. W., Eds., Electronic composition in printing. Proceedings of a Symposium held at the National Bureau of Standards June 15–16, 1967, Spec. Publ. 295 (Feb. 1968), 70 cents. (This series was formerly known as the Miscellaneous Publication Series).

Nimeroff, I., Colorimetry, Mono. 104 (Jan. 1968), 35 cents. Supersedes Circular 478.

Petersen, P. H., and Watstein, D., Shrinkage and creep in prestressed concrete, Bldg. Sci. Series 13 (Mar. 22, 1968), 15 cents.

Popenoe, C. H., and Thompson, R. C., Accessory equipment and teletypewriter modifications for remote computer consoles, Tech. Note 419 (Feb. 1968), 20 cents.

Radebaugh, R., Thermodynamic properties of He^3-He^4 solutions with applications to the He^3-He^4 dilution refrigerator, Tech. Note 362 (Dec. 29, 1967), 70 cents.

Rasberry, S. D., Margoshes, M., and Scribner, B. F., Applications of a time-sharing computer in a spectrochemistry laboratory: Optical emission and x-ray fluorescence, Tech. Note 407 (Feb. 1968), 40 cents.

Robbins, D., Ed., Disclosures on: Autoeditor—a semi-automatic copy-editing apparatus, Tech. Note 440 (Apr. 1968), 40 cents.

Roberts, A. G., Organic coatings. Properties, selection, and use, Bldg. Sci. Series 7 (Feb. 1968), $2.50.

Shelton, C. F., Spectral emission properties of NBS standard phosphor samples under photo-excitation, Tech. Note 417 (Mar. 1968), 25 cents.

Shimanouchi, T., Tables of molecular vibrational frequencies, Part 3, Natl. Std. Reference Data Series 17 (Mar. 1968), 30 cents.

Safety rules for the installation and maintenance of electric supply and communication lines, Handb. 81, Supplement 2 (Mar. 1968), 5 cents.

Standard reference materials: catalog and price list of standard materials issued by the National Bureau of Standards, Misc. Publ. 260, 1968 Edition (Jan. 31, 1968), 45 cents. (Supersedes NBS Misc. Publ. 260, 1967 Edition.)

Wegstein, J. H., A computer oriented single-fingerprint identification system, Tech. Note 443 (Mar. 1968), 25 cents.

Allan, D. W., Fey, L., Machlan, H. E., and Barnes, J. A., An ultra-precise time synchronization system designed by computer simulation, Frequency **6,** No. 1, 11–14 (Jan. 1968).

Arenhovel, H., and Hayward, E., Scattering of plane-polarized photons by the giant resonances of nuclei, Phys. Rev. **165,** No. 4, 1170–1174 (Jan. 20, 1968).

Astin, A. V., A time for action in international standardization, Mater. Res. Std. **8,** No. 5, 18–24 (May 1968).

Ausloos, P., and Lias, S. G., Gas-phase radiolysis of hydrocarbons, Book, Actions Chimique et Biologiques des Radiations, Ed. M. Haissinsky, **10,** 1 (Masson and Company, Paris, France, 1967).

Ausloos, P., and Lias, S. G., Gas-phase photolysis of hydrocarbons in the photoionization region, Rad. Res. Rev. **1,** No. 1, 75–107 (Mar. 1967).

Ausloos, P., and Lias, S. G., Photoionization of cycloalkanes in the gas phase. A study of charge transfer-processes, Book, The Chemistry of Ionization and Excitation, Eds. G. Johnson and G. Schales, pp. 77–89 (Taylor and Francis, Ltd., London, England, 1967).

Ausloos, P., Scala, A. A., and Lias, S. G., Ion-molecule reactions in the condensed-phase radiolysis of hydrocarbon mixtures. II. Cyclopentane and cyclohexane, J. Am. Chem. Soc. **89,** 3677–3683 (1967).

Balling, L. C., g_l/g_l ratios of Rb^{85} and Rb^{87}, Phys. Rev. **163,** No. 1, 114–118 (Nov. 5, 1967).

Barnes, J. A., and Allan, D. W., An approach to the prediction of coordinated universal time, Frequency **5,** No. 6, 15–20 (Nov.–Dec. 1967).

Bates, R. G., and Covington, A. K., Behavior of the glass electrode and other *p*H-responsive electrodes in biological media, Ann. N.Y. Acad. Sci. **148,** 67–80 (Feb. 1, 1968).

Bender, P. L., Radio reflection by free radicals in earth's atmosphere, Science **158,** No. 3807, 1487–1488 (Dec. 15, 1967).

Bennett, L. H., Swartzendruber, Watson, R. E., Hyperfine fields and electronic structure of CsCl-type ternary alloys of the first transition series, Phys. Rev. **165,** No. 2, 500–505 (Jan. 10, 1968).

Berger, M. J., Energy deposition in water by photons from point isotropic sources, J. Nucl. Med. Suppl. **1,** 15–25 (Feb. 1968).

Blandford, J. M., A progress report on the NBS–ARF apparel materials evaluation project, First Annual Conf. Apparel Research Foundation, Nov. 29–Dec. 1, 1967, Washington, D.C. (Apparel Research Foundation, Washington, D.C. 20036, 1967).

Bowman, R. R., Remarks on the paper "Field strength above 1 GHz: Measurement procedures for standard antennas, Proc. IEEE **56,** No. 2, 216 (Feb. 1968).

Brady, E. L., and Wallenstein, M. B., The national standard reference data system, Science **156,** No. 3776, 754–762 (May 12, 1967).

Brown, R. L. and Dittmann, S., Vibrational relaxation and quenching in the yellow nitrogen afterglow, Chem. Commun. **21,** 1144–1146 (Nov. 8, 1967).

Cassidy, E. C., and Abramowitz, S., Time-resolved spectroscopic studies of exploding wires in controlled atmospheres, Appl. Spectry. **21,** No. 6, 360–364 (Nov.–Dec. 1967).

Chamberlain, G. E., Simpson, J. A., Mielczarek, S. R., and Kuyatt, C. E., Effect of double scattering on cross-section measurements at large momentum transfer, J. Chem. Phys. **47,** No. 10, 4266–4267 (Nov. 15, 1967).

Chappell, S. E., and Sparrow, J. H., The average energy required to produce an iron pair in argon, nitrogen, and air for 1- to 5-MeV alpha particles, Rad. Res. **32,** No. 3, 383–403 (Nov. 1967).

Christ, B. W., and Giles, P. M., Metallurgical uses of the Fe^{57} mössbauer effect in metallic iron and plain carbon steels, Book, Advances in Mössbauer Methodology **3,** 37–65 (Plenum Press, Inc., New York, N.Y., Jan. 1967).

Christ, B. W., and Smith, G. V., Strengthening of polycrystalline iron by nitrogen, Trans. ASM **60,** 732–734 (1967).

Christ, B. W., and Smith, G. V., Yield and flow stress increase in pure polycrystalline iron during 600 °C treatment after wet hydrogen purification, Scripta Met. **1,** No. 3, 123–130 (1967).

Chueh, P. L., and Prausnitz, J. M., Third virial coefficients of nonpolar gases and their mixtures, AIChE J. **13,** No. 5, 896–902 (Sept. 1967).

Colwell, J. H., The heat capacity of a mixed titanate superconductor, Physics Letters **25A,** No. 8, 623–624 (Oct. 1967).

Corliss, C. H., Revision of the NBS tables of spectral-line intensities below 2450Å, Spectrochim. Acta **23B,** 117–127 (1967).

Cullen, W. C., and Boone, T. H., A thermal-shock resistance factor for bituminous built-up roofing membranes, Part 1, Roofing Siding Insulation Mag. **44,** No. 11, 30–35 (Nov. 1967); Part 2, Roofing Siding Insulation Mag. **44,** No. 12, 35–59 (Dec. 1967).

Currie, L. A., Limits for qualitative detection and quantitative determination, application to radiochemistry, Anal. Chem. **40,** No. 3, 586–593 (Mar. 1968).

Cuthill, J. R., McAlister, A. J., Williams, M. L., Watson, Phys. Rev. **164,** No. 3, 1006–1007 (Dec. 15, 1967).

Damburg, R. J., and Geltman, S., Excitation of $n=2$ states in hydrogen by electron impact, Phys. Rev. Letters **20,** No. 10, 485–487 (Mar. 4, 1968).

Daney, D. E., and Mann, D. B., Quality determination of liquid-solid hydrogen mixtures, Cryog. **7,** No. 5, 280–285 (Oct. 1967).

deWit, R., Thermodynamic force on a dislocation, J. Appl. Phys. **39,** No. 1, 137–141 (Jan. 1968).

Dibeler, V. H. and Liston, S. K., Mass-spectrometric study of photoionization. VIII. Dicyanogen and the cyanogen halides, J. Chem. Phys. **47,** No. 11, 4548–4555 (Dec. 1, 1967).

Dickson, G., and Oglesby, P. L., Elastic constants of dental amalgam, J. Dental Res. **46,** No. 6, Part 2, 1475 (Nov.–Dec. 1967).

DiMarzio, E. A., Some contributions to the kinetics of growth and multicomponent chains with application to the problems of ciliation and fractionation in polymer crystallization, J. Chem. Phys. **47,** No. 9, 3451–3469 (Nov. 1, 1967).

Eberhard, J. P., Systems and design–an extrapolation to 2000 A.D., Mater. Res. Std. **8,** No. 5, 12–17 (May 1968).

Eberhard, J. P., Schofer, R. E., The role of technology in developing future transportation systems, Proc. Analysis and Control of Traffic Flow Symp., Detroit, Michigan, Jan. 9–10, 1968, pp. 1–4 (Society of Automotive Engineers, Inc., New York, N.Y., 1968).

Fatiadi, A. J., Acetic anhydride phosphoric acid as an acetylating agent, Carbohydrate Res. **6,** 237–240 (1968).

Fatiadi, A. J., Stable radicals obtained by treatment of azulene with periodic acid and other oxidants, Chem. Commun. **8,** 456–458 (Apr. 24, 1968).

Fine, J., and Scheer, M. D., Positive and negative self-surface ionization of molybdenum, J. Chem. Phys. **47,** No. 10, 4267–4268 (Nov. 15, 1967).

Franklin, A. D., Born model calcuation of enthalpies of solution in CaF_2 J. Am. Ceramic Soc. **50,** No. 12, 648–652 (Dec. 1967).

Gross, D., Loftus, J. J., Robertson, A. F., Method for measuring smoke from burning materials, Am. Soc. Testing Mater. Spec. Tech. Publ. **422,** 166–204 (1967).

Hafner, H., Simpson, J. A., and Kuyatt, C. E., Comparison of the spherical deflector and the cylindrical mirror analyzers, Rev. Sci. Instr. **39,** No. 1, 33–35 (Jan. 1968).

Haller, W., Correlation between chromatographic and diffusional behaviour of substances in beds of pore controlled glass. Contribution to the mechanism of steric chromatography, J. Chromatog. **32,** 676–684 (1968).

Haller, W., Virus isolation with glass of controlled pore size: MS2 bacteriophage and kilham virus, Virology **33,** No. 4, 740–743 (Dec. 1967).

Hamer, W. J., A Joule centennial, J. Chem. Educ. **45,** No. 2, 123–125 (Feb. 1968).

Hanley, H. J. M., Thermodynamics of transport phenomena in membrane systems, J. Chem. Educ. **44,** No. 12, 717–719 (Dec. 1967).

Hanley, H. J. M., and Childs, G. E., Discrepancies between viscosity data for simple gases, Science **159,** No. 3819, 1114–1117 (Mar. 8, 1968).

Hetzer, H. B., Robinson, R. A., and Bates, R. G., Conventional pa_H values for buffer solutions of piperazine phosphate from 0° to 50° C, Anal. Chem. **40,** 634–636 (Mar. 1968).

Holt, H. K., Frequency-correlation effects in cascade transitions involving stimulated emission, Phys. Rev. Letters **19,** No. 22, 1275–1277 (Nov. 27, 1967).

Holt, H. K., Observation of the effect of frequency correlations on a cascade transition, Phys. Rev. Letters **20,** No. 9, 410–412 (Feb. 26, 1968).

Hudson, R. P., Generation of matrix elements of angular-momentum operators, J. Opt. Soc. Am. **57,** No. 12, 1552–1553 (Dec. 1967).

Hummer, D. G., Non-coherent scattering—III. The effect of continuous absorption on the formation of spectral lines, Monthly Notices Roy. Astron. Soc. **138,** No. 1, 73–108 (1968).

Ito, J., A new yttrium magnesium silicate garnet, $Y_6Mg_5Si_3O_{24}$ and its rare earth and nickel analogues, Mater. Res. Bull. **2,** 1093–1098 (1967).

Jensen, M. W., Milk meters, farm milk tank testing, and plastic containers for milk, Proc. 31st Annual Meeting International Association of Milk Control Agencies, Biloxi, Mississippi, Oct. 23–25, 1967, pp. 26–31 (1968).

Jespersen, J. L., Kamas, G., and Morgan, A. H., A proposed ranging system with application to VLF timing, IEEE Trans. Instr. Meas. **IM-16,** No. 4, 282–285 (Dec. 1967).

Johannesen, R. B., Brinckman, F. E., and Coyle, T. D., Nuclear magnetic resonance studies of inorganic fluorides. V. Fluorosilanes, J. Phys. Chem. **72,** 660–667 (1968).

Kamper, R. A., Millidegree noise thermometry, Proc. Symp. Physics of Superconducting Devices, University of Virginia, Apr. 28–29, 1967, pp. M–1 through M–5 (Office of Naval Research, Wash., D.C., 1968).

Klein, R., and Scheer, M. D., Mechanism of O(^{3}P) addition to condensed films. II. Propene, 1-butene, and their mixtures, J. Phys. Chem. **72,** No. 2, 616–622 (Feb. 1968).

Knight, J. M., O'Connell, J. S., and Prats, F., Two- and three-body photodisintegration cross sections of ^{3}H and ^{3}He, Phys. Rev. **164,** No. 4, 1354–1359 (Dec. 20, 1967).

Kolbenstvedt, H., Energy transfer in the collision of electron beams, Phys. Rev. **163,** No. 1, 112–114 (Nov. 5, 1967).

Kolbenstvedt, H., Simple theory for K-ionization by relativistic electrons, J. Appl. Phys. **38,** No. 12, 4785–4787 (Nov. 1967).

Krause, R. F., Jr., and Douglas, T. B., The vapor pressure, vapor dimerization, and heat of sublimation of aluminum fluoride, using the entrainment method, J. Phys. Chem. **72,** No. 2, 475–481 (Feb. 1968).

Kuriyama, M., Distortion correction in anomalous absorption coefficients, Phys. Stat. Sol. **24,** 743–748 (1967).

Kuriyama, M., Theory of X-ray diffraction by a distorted crystal, J. Phys. Soc. Japan **23,** No. 6, 1369–1379 (Dec. 1967).

Lafferty, W. J., Direct *l*-type doubling transitions in some axially symmetric molecules, J. Mol. Spectry. **25,** No. 8, 359–364 (Mar. 1968).

Landgrebe, A. R., McSharry, W. O., and Cefola, M., The radiometric titration of trace amounts of zinc, Intern. J. Appl. Radiation Isotopes **19,** 1, 23–26 (1968).

Landgrebe, A. R., Rodriguez-Pasques, R. H., and Schima, F. J., The rapid radiochemical separation of radioactive praseodymium from radioactive cerium, Intern. J. Appl. Radiation Isotopes **19,** No. 2, 147–149 (1968).

LeLevier, R. E., and Branscomb, L. M., Ion chemistry governing mesospheric electron concentrations, J. Geophys. Res., Space Physics **73,** No. 1, 27–41 (Jan. 1, 1968).

Madey, T. E., and Yates, J. T., Jr., Work function studies: chemisorption of diatomic molecules on single-crystal tungsten, Nuovo Cimento Suppl. Series I, **5,** No. 1, 483–505 (1967).

Maki, A. G., Jr., and Lide, D. R., Jr., Microwave and infrared measurements on HCN and DCN; observations on *l*-type resonance doublets, J. Chem. Phys. **47,** No. 9, 3206–3210 (Nov. 1, 1967).

Mann, R. H., and Maryott, A. A., Dipole moment of Co(CO)3NO from the nonresonant microwave absorption of the vapor, J. Chem. Phys. **47,** No. 10, 4275–4276 (Nov. 15, 1967).

Manson, S. T., and Cooper, J. W., Photo-ionization in the soft x-ray range: Z dependence in a central-potential model, Phys. Rev. **165,** No. 1, 126–138 (Jan. 5, 1968).

Marantz, S., and Armstrong, G. T., Heats of combustion of transstilbene and trans-2,2′,4,4′,6,6′-hexanitrostilbene (HNS), J. Chem. Eng. Data **13,** No. 1, 118–121 (Jan. 1968).

Marshak, H., Langsford, A., Wong, C. Y., and Tamura, T., Total neutron cross section of oriented ^{165}Ho from 2 to 135 MeV, Phys. Rev. Letters **20,** No. 11. 554–558 (Mar. 11, 1968).

Marzetta, L. A., Incorrect usage of exact closed-loop voltage gain formula in operational amplifiers, Analog Dialogue Letter **2,** No. 1, (Mar. 1968).

Maximon, L. C., and Tzara, C., Influence of the radiative background on muon and electron scattering from nuclei, Physics Letters **26B,** No. 4, 201–203 (Jan. 22, 1968).

May, L., Spijkerman, J. J., Mössbauer spectroscopy, Chemistry **40,** 14–17 (Dec. 1967).

Mielenz, K. D., Nefflen, K. F., Rowley, W. R. C., Wilson, D. C., and Engelhard, E., Reproducibility of helium-neon laser wavelengths at 633 nm, Appl. Opt. **7,** No. 2, 289–293 (Feb. 1968).

Milligan, D. E., and Jacox, M. E., Infrared and ultraviolet spectroscopic study of the products of the vacuum-ultraviolet photolysis of methane in Ar and N_2 matrices. The infrared spectrum of the free radical CH_3, J. Chem. Phys. **47,** No. 12, 5146–5156 (Dec. 15, 1967).

Milligan, D. E., and Jacox, M. E., Matrix-isolation study of the infrared and ultraviolet spectra of the free radical NCO, J. Chem. Phys. **47,** No. 12, 5157–5168 (Dec. 15, 1967).

Moore, C. E., Annual report on spectroscopy, Astron. J. **72,** No. 9, 1117–1118 (1967).

Moore, C. E., Necrology: Carl C. Kiess, J. Opt. Soc. Am. **58,** No. 2, 292–293 (Feb. 1968).

O'Connell, J. S., and Prats, F., Photodisintegration of the trinucleon system in a separable potential model, Physics Letters **26B,** No. 4, 197–200 (Jan. 22, 1968).

Okabe, H., and Lenzi, M., Photodissociation of NH_3 in the vacuum ultraviolet, J. Chem. Phys. **47,** No. 12, 5241–5246 (Dec. 15, 1967).

Pella, P. A., Landgrebe, A. R., DeVoe, J. R., and Purdy, W. C., Differential controlled-potential coulometry utilizing substoichiometric radioisotope dilution, Anal. Chem. **39,** 1781–1785 (Dec. 1967).

Pfeiffer, E. R., and Schooley, J. F., Effect of stress on the superconductive transition temperature of strontium titanate, Phys. Rev. Letters **19,** No. 14, 783–785 (Oct. 2, 1967).

Preston, G. T., Chapman, T. W., and Prausnitz, J. M., Transport properties of cryogenic liquids and their mixtures, Cryog. **7,** No. 5, 274–279 (Oct. 1967).

Prince, E., and Rush, J. J., Many disciplines unit to study solid structure and dynamics, Phys. Today **21,** No. 2, 95–99 (Feb. 1968).

Pytte, E., and Bennett, H. S., Ultrasonic attenuation in the Heisenberg paramagnet. II. Antiferromagnets, Phys. Rev. **164,** No. 2, 712–715 (Dec. 10, 1967).

Rasberry, S. D., Caul, H. J., and Yezer, A., X-ray fluorescence analysis of silver dental alloys with correction for a line interference, Spectrochim. Acta **23B,** 345–351 (Mar. 1968).

Risley, A. S., Parallel pump susceptibility of YIG under cw drive conditions, Physics Letters **25A,** No. 6, 471–472 (Sept. 25, 1967).

Ronn, A. M., and Lide, D. R., Jr., Infrared-microwave double resonance using a CO_2 laser, J. Chem. Phys. **47,** No. 9, 3669–3670 (Nov. 1, 1967).

Scala, A. A., and Ausloos, P., Condensed-phase photolysis and radiolysis of 2-methylbutane, J. Chem. Phys. **47,** No. 12, 5129–5139 (Dec. 15, 1967).

Schima, F. J., and Hutchinson, J. M. R., Energy of the isomeric transition in ^{109}Ag, Nucl. Phys. **A102,** 667–672 (1967).

Schofer, R. E., and Levin, B. M., The urban transportation planning process, Socio-Econ. Plan. Sci. **1,** 185–197 (Pergamon Press Ltd., London, England, 1967).

Simpson, J. A., Electron guns, Book, Methods of Experimental Physics, Chapter, Sources of Atomic Particles, **4,** 84–95 (Academic Press Inc., New York, N.Y., 1967).

Simpson, J. A., Special sources of monoenergetic electrons, Book, Methods of Experimental Physics, Volume 4, Atomic and Electron Physics, Chapter, Sources of Atomic Particles, Section 1.1.7, pp. 124–135 (Academic Press Inc., New York, N.Y., 1967).

Sparks, L. L., and Powell, R. L., Metals characterization by low-temperature thermoelectric methods, Meas. Data **1,** No. 5, 89–96 (Sept.–Oct. 1967).

Spijkerman, J. J., Application of Mössbauer spectroscopy to structure analysis (Proc. Second Symp. on Low Energy X- and Gamma Sources and Applications, University of Texas, Austin, Texas, Mar. 27–29, 1967), Oak Ridge National Laboratory–IIC–10, pp. 85–100 (1967).

Spijkerman, J. J., The Mössbauer chemical shift in tin chemistry, Advan. Chem. Ser. **68,** 105–112 (1968).

Swanson, N., Characteristic energy-loss spectra and -Im(1/ε) for amorphous and polycrystalline Al_2O_3, Phys. Rev. **165,** No. 3, 1067–1070 (Jan. 15, 1968).

Swartzendruber, L. J., and Bennett, L. H., The effect of Fe on the corrosion rate of copper rich Cu-Ni alloys, Scripta Metallurgica **2,** 93–98 (1968).

Taylor, L. S., Responsibilities of the physician in his use of radiation, Rev. Mex. Radiol. **XVIII,** No. 69, 22–31 (Jan.–Feb. 1964).

Van Blerkom, D., and Hummer, D. G., The ionization structure of planetary nebulae-VI. The Lyman continuum problem, Monthly Notices Roy. Astron. Soc. **137,** 353–374 (1967).

Vriens, L., Simpson, J. A., and Mielczarek, S. R., Tests of born approximations: differential and total 2^3S, 2^1P, and 2^1S cross sections for excitation of He by 100- to 400-eV electrons, Phys. Rev. **165,** No. 1, 7–15 (Jan. 5, 1968).

Weiss, A. W., Theoretical electron affinities for some of the alkali and alkaline-earth elements, Phys. Rev. **166,** No. 1, 70–74 (Feb. 5, 1968).

Weiss, A. W., Theoretical multiplet strengths for Mg I, Al II, and Si III, J. Chem. Phys. **47,** No. 9, 3573–3578 (Nov. 1, 1967).

Wells, J. S., Matarrese, L. M., and Sukle, D. J., Electron spin resonance in single crystals of anhydrous copper sulfate, J. Chem. Phys. **47,** No. 7, 2259–2262 (Oct. 1, 1967).

Whittaker, J. K., Instability and decoupling in nuclear electronics, Nucl. Instr. Methods **57,** No. 1, 156 (Dec. 1967).

Wilcox, R. M., Some thoughts on Fitzgerald's particle waves, J. Acoust. Soc. Am. **42,** No. 3, 678–679 (Sept. 1967).

Yakowitz, H., and Heinrich, K. F. J., Quantitative electron probe microanalysis: Absorption correction uncertainty, Mikrochim. Acta **1,** 182–200 (1968).

Yates, J. T., Jr., Madey, T. E., and Payn, J. K., Desorption by electron impact: carbon monoxide, nitric oxide and oxygen on tungsten, Nuovo Cimento Suppl. Series I, **5,** No. 2, 558–581 (1967).

**Publications for which a price is indicated are available by purchase from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402 (foreign postage, one-fourth additional). The NBS nonperiodical series are also available from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Va. 22151. Reprints from outside journals and the NBS Journal of Research may often be obtained directly from the authors.*

U.S. GOVERNMENT PRINTING OFFICE : 1968 O—312-532

UNITED STATES
GOVERNMENT PRINTING OFFICE
DIVISION OF PUBLIC DOCUMENTS
WASHINGTON, D.C. 20402

OFFICIAL BUSINESS

POSTAGE AND FEES PAID
U.S. GOVERNMENT PRINTING OFFICE

JOURNAL OF RESEARCH of the National Bureau of Standards Vol. 72B, No. 3 July–September 1968
B. Mathematical Sciences

MIAMI UNIVERSITY LIBRARY

Contents

Page

Interaction in multidimensional contingency tables: An information theoretic approach. H. H. Ku and S. Kullback. 159

On the coupling of longitudinal and transverse waves in a linear three-element viscoelastic string subjected to transverse impact. Jack C. Smith and Jeffrey T. Fong. 201

Allocating service periods to minimize delay time. W. A. Horn. 215

The second orthogonality conditions in the theory of proper and improper rotations. I. Derivation of the conditions and of their main consequences. Harry Gelman. 229

Thickness and connectivity in graphs. Arthur M. Hobbs and J. W. Grossman. 239

Publications of the National Bureau of Standards. 245

Library of Congress Catalog Card Number: 62–4414

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Price 75c (single copy). Subscription price: $2.25 a year; 50c additional for foreign mailing.

UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1968